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Optimal Designs of Spin- and Majorana Qubit Devices

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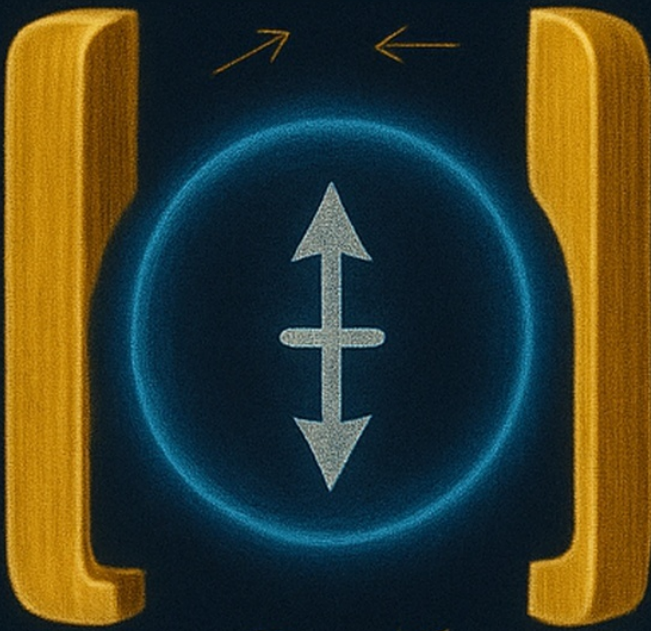
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Optimal designs of spin- and Majorana qubit devices



Sathish Kumar
Kuppuswamy

OPTIMAL DESIGNS OF SPIN- AND MAJORANA QUBIT DEVICES

OPTIMAL DESIGNS OF SPIN- AND MAJORANA QUBIT DEVICES

Dissertation

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by

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Front & Back: Front cover shows two qubit designs — a Majorana qubit on the left with paired orange ends connected by blue curves, and a spin qubit on the right represented by a blue sphere inside golden electrostatic gates. Two arrows pointing opposite inside the sphere represent electron spin. The background and back cover features random golden arrows symbolizing electron noise, and the gates partially shield the qubits.

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To my wife and parents.

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SUMMARY

The realization of scalable, fault-tolerant quantum computing hinges on the successful development of device platforms, materials, and architectures capable of supporting large-scale, error-resilient quantum operations. Achieving this goal requires overcoming both physical noise and architectural inefficiencies, while maintaining high-fidelity control over qubit states. This thesis investigates two leading qubit implementations—spin qubits and Majorana qubits—and introduces simulation-based methodologies designed to accelerate their design cycles and enhance their performance.

Spin qubits encode quantum information in the spin states of electrons confined within semiconductor quantum dots. Their key advantage lies in leveraging mature semiconductor fabrication technology, which allows for sophisticated, highly integrated gate architectures. However, spin qubits are inherently vulnerable to decoherence caused by charge noise, crystal defects, and fluctuations in the surrounding electromagnetic environment. These effects can disrupt qubit initialization and manipulation, posing a fundamental challenge for fault-tolerant operation.

In contrast, Majorana qubits are formed from spatially separated yet quantum-mechanically entangled Majorana quasiparticles, whose non-Abelian exchange statistics provide topological protection against certain forms of decoherence. This intrinsic robustness makes them attractive candidates for long-lived quantum information storage. Nevertheless, the practical realization of controllable Majorana devices remains difficult, with major experimental hurdles in engineering gate structures capable of initializing and braiding the quasiparticles reliably.

The core objective of this thesis is to develop simulation techniques for rapid exploration and optimization of gate designs, thereby mitigating the inefficiencies of purely experimental, trial-and-error approaches. In chapter 2, we introduce the hybrid kernel polynomial method, which combines sparse diagonalization of the most relevant low-energy states with the kernel polynomial method to efficiently include contributions from higher-energy states. This hybrid approach enables accurate evaluation of thermodynamic quantities and the construction of effective perturbative models in parameter regimes where neither method alone is sufficient. Its versatility is demonstrated through applications to the calculation of supercurrent and inductance in Josephson junctions, the interaction of spin qubits in two-dimensional electron gases, and the effective band structure of semiconductor nanowires.

Following conceptual design, we applied numerical optimization using cost functions specifically tailored to each qubit platform. For spin qubits, the cost function incorporates the chemical potentials of the dots, interdot tunnel couplings, and quantum dot positions—parameterized via Wannier centers. We chose the weighting coefficients for each parameter carefully to promote rapid and stable convergence during optimization.

In chapter 3, we studied the impact of disorder on gate coupling strengths in spin qubit devices. We developed a simulation framework to quantify how electrostatic gate voltages

couple to the effective device Hamiltonian in the presence of material and fabrication-induced disorder. Comparisons with experimental data revealed strong agreement within the expected disorder-induced variance. To illustrate the adaptability of the framework, it is also applied to alternative non-planar device geometries inspired by FinFET technology, highlighting its potential for guiding the design of unconventional architectures.

In chapter 4, we designed a Majorana trijunction, a critical building block for braiding operations that demonstrate non-Abelian exchange statistics. The design challenge lies in achieving strong coupling between desired pairs of Majorana modes while suppressing unwanted couplings, all without closing the topological gap. We used an optimization procedure to identify suitable operational regimes in a multi-dimensional voltage space. Simulated braiding experiments confirmed that adiabatic coupling sequences can be implemented while preserving topological protection. The robustness of braiding is further evaluated across different trijunction geometries and levels of disorder.

In summary, this thesis presents a comprehensive simulation framework for quantum device gate design. By applying these techniques to both spin and Majorana qubit architectures, we aim to shorten the design iteration cycles, improve device performance predictions, and contribute to the broader goal of realizing experimentally feasible, scalable, and fault-tolerant quantum computing.

SAMENVATTING

De realisatie van schaalbare, fouttolerante kwantumcomputers is afhankelijk van de succesvolle ontwikkeling van apparaatplatforms, materialen en architecturen die in staat zijn grootschalige, foutbestendige kwantumoperaties te ondersteunen. Het bereiken van dit doel vereist het overwinnen van zowel fysische ruis als architectonische inefficiënties, terwijl een hoge-fideliteitscontrole over qubit-toestanden behouden blijft. Dit proefschrift onderzoekt twee toonaangevende qubit-implementaties—spin qubits en Majorana qubits—en introduceert simulatiemethoden die zijn ontworpen om hun ontwerpcyclus te versnellen en de prestaties te verbeteren.

Spin qubits coderen kwantuminformatie in de spin-toestanden van elektronen die opgesloten zijn in halfgeleider-quantumdots. Hun belangrijkste voordeel ligt in het benutten van volwassen halfgeleiderfabricagetechnologie, die verfijnde en sterk geïntegreerde poortarchitecturen mogelijk maakt. Spin qubits zijn echter van nature gevoelig voor decoherentie veroorzaakt door ladingsruis, kristaldefecten en fluctuaties in de omliggende elektromagnetische omgeving. Deze effecten kunnen de initiatie en manipulatie van qubits verstoren, wat een fundamentele uitdaging vormt voor fouttolerante werking.

Daarentegen worden Majorana qubits gevormd door ruimtelijk gescheiden maar kwantummechanisch verstrengelde Majorana-quasideeltjes, waarvan de non-Abelian uitwisselingsstatistieken topologische bescherming bieden tegen bepaalde vormen van decoherentie. Deze intrinsieke robuustheid maakt ze aantrekkelijke kandidaten voor langdurige opslag van kwantuminformatie. Niettemin blijft de praktische realisatie van bestuurbare Majorana-apparaten moeilijk, met grote experimentele uitdagingen bij het ontwerpen van poortstructuren die deze quasipartikels betrouwbaar kunnen initialiseren en vlechten.

Het centrale doel van dit proefschrift is het ontwikkelen van simulatietechnieken voor snelle verkenning en optimalisatie van poortontwerpen, waardoor de inefficiënties van louter experimentele trial-and-error-benaderingen worden verminderd. In hoofdstuk 2 introduceren we de hybride kernelpolynoommethode, die de sparse-diagonalisatie van de meest relevante laagenergiestanden combineert met de kernelpolynoommethode om bijdragen van hoger-energiestanden efficiënt te integreren. Deze hybride aanpak maakt nauwkeurige berekeningen mogelijk van thermodynamische grootheden en de constructie van effectieve perturbatieve modellen in parameterruimten waar geen van beide methoden afzonderlijk toereikend is. De veelzijdigheid wordt aangetoond via toepassingen in de berekening van superstroom en inductantie in Josephson-juncties, de interactie van spin qubits in tweedimensionale elektrongassen en de effectieve bandstructuur van halfgeleider-nanodraden.

Na het conceptuele ontwerp hebben we numerieke optimalisatie toegepast met behulp van kostenfuncties die specifiek zijn afgestemd op elk qubitplatform. Voor spin qubits omvat de kostfunctie de chemische potentialen van de dots, tunnelkoppelingen tussen dots en de posities van de quantumdots—geparametriseerd via Wannier-centra.

We hebben de weegcoëfficiënten voor elke parameter zorgvuldig gekozen om snelle en stabiele convergentie tijdens de optimalisatie te bevorderen.

In hoofdstuk 3 hebben we de impact van wanorde op de gate-koppelingssterkte in spin qubit devices bestudeerd. We hebben een simulatieframework ontwikkeld om te kwantificeren hoe elektrostatistische gate-spanningen koppelen aan de effectieve device-Hamiltoniaan in aanwezigheid van materiaal- en fabricage-geïnduceerde wanorde. Vergelijkingen met experimentele gegevens tonen een sterke overeenstemming binnen de verwachte, door wanorde veroorzaakte variatie. Om de aanpasbaarheid van het framework te illustreren, hebben we het toegepast op alternatieve niet-planaire device-geometrieën geïnspireerd op FinFET-technologie, waarmee we de potentie ervan voor het ontwerpen van onconventionele architecturen hebben benadrukt.

In hoofdstuk 4 hebben we een Majorana-trijunctie ontworpen, een cruciale bouwsteen voor braiding-bewerkingen die non-Abelian uitwisselingsstatistieken demonstreren. De ontwerputdaging ligt in het realiseren van sterke koppeling tussen gewenste paren van Majorana-modi, terwijl ongewenste koppelingen worden onderdrukt, zonder de topologische kloof te sluiten. We hebben een optimalisatieprocedure gebruikt om geschikte operationele regimes in een multidimensionale spanningsruimte te identificeren. Gesimuleerde vlecht-experimenten bevestigen dat adiabatische koppelingssequenties kunnen worden uitgevoerd met behoud van topologische bescherming. De robuustheid van het vlechten wordt verder geëvalueerd voor verschillende drieverbindingsgeometrieën en niveaus van wanorde.

Samenvattend presenteert dit proefschrift een uitgebreid simulatiekader voor het ontwerp van kwantumapparaatpoorten. Door deze technieken toe te passen op zowel spin- als Majorana-qubitarchitecturen, streven we ernaar de ontwerpiteratiecycli te verkorten, de prestatievoorspellingen van devices te verbeteren en bij te dragen aan het bredere doel van het realiseren van experimenteel haalbare, schaalbare en fouttolerante quantumcomputing.

1

INTRODUCTION

1.1. PREFACE

Traditional computers face a significant challenge when dealing with large inputs, as their processing time grows exponentially with the size of the problem. In contrast, quantum computers are exponentially faster in solving certain problems, thanks to the unique ability of quantum mechanics to harness superposition. Unlike classical computers, which operate in a binary system (0 or 1), quantum computers rely on quantum bits (qubits) that can exist in multiple states simultaneously, allowing them to explore a vast solution space in a single operation. In a quantum system, qubits exist as complex vectors in a two-dimensional Hilbert space, represented by coefficients α and β ,

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle. \quad (1.1)$$

By rotating the basis states around the Bloch sphere as illustrated in Fig. 1.1, the qubits can be placed in a superposition state. This property enables quantum algorithms to process

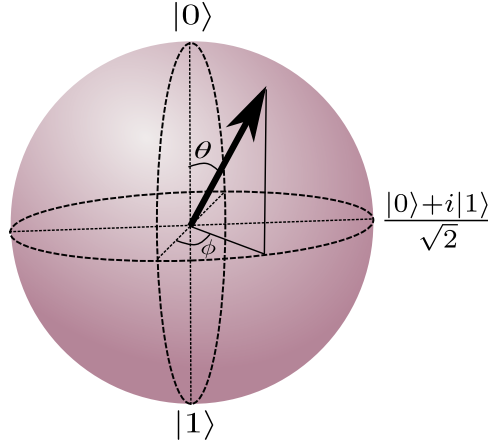


Figure 1.1: Bloch sphere with the qubit basis states represented as $|0\rangle$ and $|1\rangle$ on its north and south poles respectively. An arbitrary qubit state is represented by $\cos(\theta/2)|0\rangle + \exp(i\phi)\sin(\theta/2)|1\rangle$ with $\phi \in [0, 2\pi]$ and $\theta \in [0, \pi]$

multiple basis states simultaneously, resulting in parallelism. Quantum algorithms that take advantage of this feature can factorize large numbers into their prime components, search large unstructured databases, and simulate complex quantum systems. These applications have practical uses in cryptography, optimization, and quantum simulation.

Several platforms have been proposed to build a quantum computer, including superconducting circuits, trapped ions, and nitrogen-vacancy centers in diamond, among others. This thesis will focus on two additional platforms: spin qubits and Majorana qubits. Spin qubits are designed to work with quantum dots, while Majorana qubits operate with nanowires. Both types of qubits are semiconductor structures that emerge from a two-dimensional electron gas (2DEG) confined within a semiconductor heterostructure.

While quantum computers rely on the unique properties of quantum mechanics, they still rely on classical electronics in many areas, such as controlling quantum operations,

correcting errors, and interacting with the outside world. A key example of this is using classical electrostatic gates to create quantum bits. By applying voltages to metal gates deposited on top of a semiconductor heterostructure, the charge density in the 2DEG can be varied, affecting the chemical potential. By carefully designing the gates, it is possible to create nanowires or quantum dots by varying the chemical potential relative to the overall Fermi energy.

1.2. SPIN QUBITS

Electrons possess an intrinsic property known as spin, which has two distinct states: up-state($|\uparrow\rangle$) and down-state($|\downarrow\rangle$). These states can exist in a superposition, as represented by Eq. 1.1, allowing for the encoding of quantum information. This two-level system is a fundamental characteristic of a qubit, and it forms the basis of spin qubits.

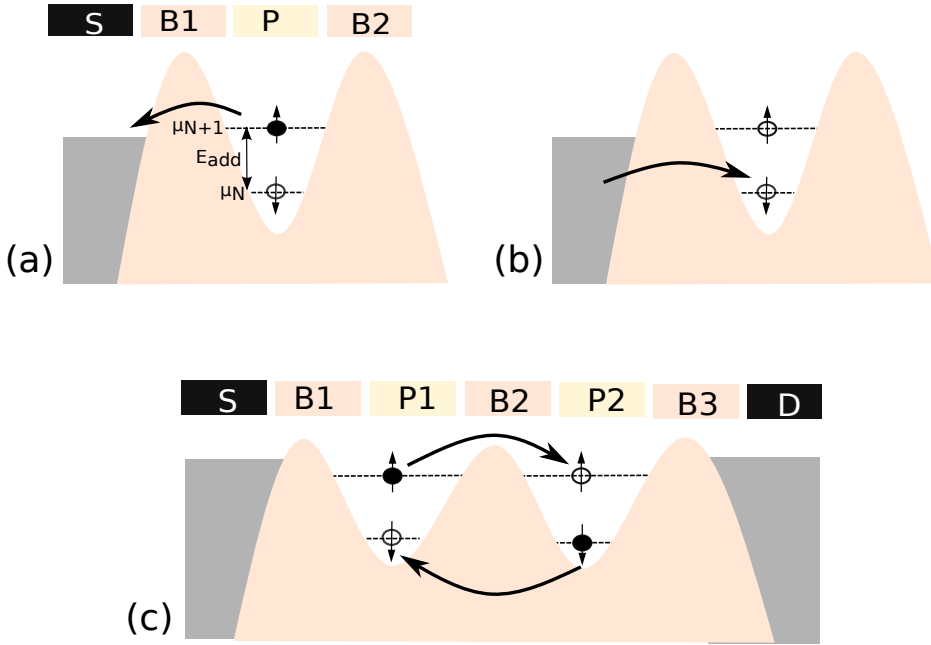


Figure 1.2: Spin qubits. (a) Charge island with two discrete energy levels for the spin-down electron (bottom) and spin-up electron (top). Energy levels are represented by chemical potential which can be controlled by gate voltages (B1, P, and B2). An electron can tunnel from the quantum dot to the source Fermi reservoir (S) as shown in (a) and back to the island as shown in (b). This marks the first step of the qubit operation — initialization. Afterward, the electron spin vector can be rotated around the Bloch sphere by applying magnetic or electric field. An electron cannot hop from a lower to higher energy state without supplying additional energy denoted by E_{add} . (c) Two charge islands with one electron each define the basis for singlet-triplet qubits.

1.2.1. QUANTUM DOTS

Spin qubits are particularly well-suited for implementation using electrons confined within semiconductor quantum dots. Quantum dots are zero-dimensional semiconductor systems that spatially confine an electron (or hole) wavefunction in all three dimensions. Their typical size is on the order of a few tens of nanometers (nm) which is comparable to the de Broglie wavelength of electrons confined within them. As a result, the energy of confined electrons is quantized similar to that of atoms and they are called *artificial atoms*. The quantized energy spectrum enables electrons to be added or removed from the quantum dot in integer numbers, a process that requires additional energy E_{add} , as shown in Fig. 1.2(a). The energy required to add an extra electron to a quantum dot is

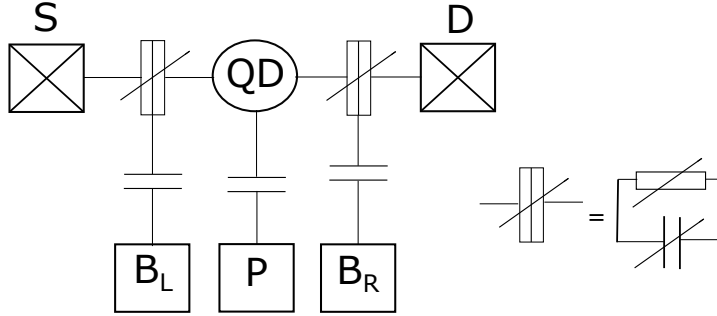


Figure 1.3: Quantum dot is connected to the source (S) and drain (D) reservoir with a variable capacitor. Dot chemical potential is tuned by a plunger (P) gate and tunnel barrier to the reservoir controlled by barrier gates (B_L and B_R).

the sum of two components: the classical charging energy E_C and quantum-mechanical orbital energy E_{orb} . E_C is the energy required to overcome the coulomb repulsions between the added electron and the existing electrons. This energy can be modeled using the constant interaction model, which assumes that the Coulomb interactions can be characterized by variable capacitances connected to the dot, as shown in Fig. 1.3. Therefore, the discrete single-particle energy spectrum of quantum dots does not depend on the interactions. E_C is defined as e^2/C where e is the electron charge and C is the sum of all dot capacitances. E_{orb} is the energy difference between the discrete single-electron states and is related to the size of the quantum dot as $\frac{\hbar^2}{m^* a^2}$ where m^* is the effective mass of semiconductor and a is the size of the quantum dot. Fig. 1.2 and Fig. 1.3 illustrates a quantum dot as a charge island and a circle, respectively. The size of the quantum dot can be controlled by adjusting the width of the plunger and barrier gates, which are carefully designed to provide a high degree of control over the quantum dot energy spectrum.

As a quantum mechanical object, electrons can tunnel from one quantum dot to another depending on the height and width of the potential barrier, as well as the energy of the discrete states in the dots. The plunger and barrier gates can be tuned to control these elements. When electrons tunnel between dots, the lowest occupied states in each dot hybridize, leading to an anti-crossing phenomenon in the energy spectrum, as shown in Fig. 1.4(c). The electron occupation of a double quantum dot system can be visualized by a charge stability diagram, as depicted in Fig. 1.4(b). Each hexagonal plane

in the diagram represents a constant occupation number, while the lines separating the planes from their neighbors denote a transition of exactly one electron between dots. Hybridization splits the points at which charge transition lines meet into two, resulting in a triple point. The tilted lines in the diagram give it a honeycomb pattern, which is typical for a charge stability diagram. When tunneling is disabled, changing the voltage of gate V_{G1} alone results in vertical charge transition lines, while the regions in between them have a fixed charge configuration. Similarly, tuning V_{G2} for a fixed V_{G1} produces horizontal lines resulting in a rectangular 2D array. In practice, the dots are influenced by changing the gate voltage of the neighboring dot, which is denoted by cross-capacitances between gates. This tilts the charge transition lines, as shown in Fig. 1.4(b).

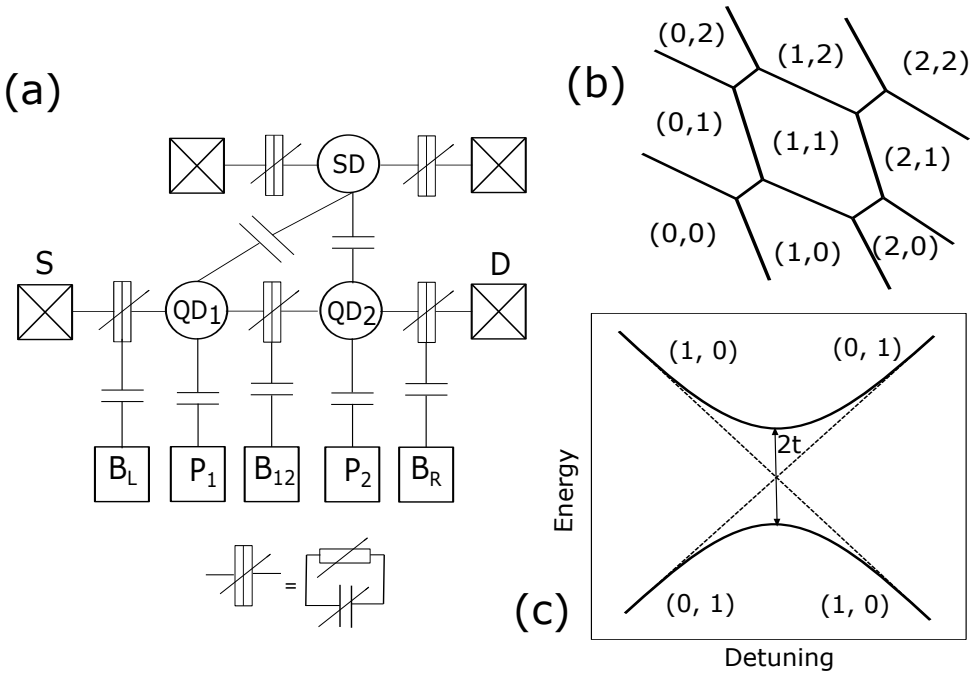


Figure 1.4: (a) Two quantum dots connected to a sensing dot are used to detect charge transfer and infer the charge occupation of the dots. (b) The charge stability diagram shows a honeycomb pattern, with the numbers in the round brackets indicating the charge occupation of each dot. (c) The energy diagram as a function of charge detuning, corresponding to a change in the plunger gate voltage, is depicted. The dashed lines represent the classical regime with no tunnel coupling, whereas the solid lines represent the case with tunnel coupling (t). The charge hybridization leads to anti-crossing, resulting in an energy separation of $2t$.

A one-dimensional array of many quantum dots has been developed to demonstrate the scalability of semiconductor-based qubits and to explore the quantum phases of matter [1]. The dynamics of electrons confined in this array are governed by several key parameters, including:

1. The on-site potential energy offset ϵ , which represents the energy difference between the quantum dots.

2. The interdot tunnel coupling t_{ij} , which describes the transfer of electrons between adjacent quantum dots.
3. The on-site U , which represents the energy cost of adding an extra electron to a quantum dot.
4. The inter-site Coulomb interactions V_{ij} , which describe the electrostatic repulsion between electrons on neighboring quantum dots.

These parameters can be effectively combined using lattice models, such as the Fermi-Hubbard model [2], which can help us understand the behavior of the electrons in the quantum dot array.

$$H = - \sum_i \epsilon_i n_i - \sum_{\langle i,j \rangle, \sigma} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.) + \sum_i \frac{U_i}{2} n_i (n_i - 1) + \sum_{i,j} V_{ij} n_i n_j, \quad (1.2)$$

where $c_{i\sigma}^\dagger$ and $c_{j\sigma}$ are the site-and-spin-specific electron creation and annihilation operators. $n_i = \sum_\sigma c_{i\sigma}^\dagger c_{i\sigma}$ is the occupation number of the i^{th} dot.

1.2.2. QUBIT PROPOSALS

According to Loss-Divincenzo's proposal [3] for spin qubits, the spin states of a single electron confined in a quantum dot are controlled by electrostatic gates. The energy levels of a single electron are spin-degenerate, with two-fold degeneracy. By applying a static magnetic field B , Zeeman coupling is introduced, which lifts the spin degeneracy and results in an energy-splitting

$$E_Z = g\mu_B B, \quad (1.3)$$

where g is the Landé g -factor and μ_B is the Bohr magneton. The two spin eigenstates, located on opposite sides of the Bloch sphere, can be coherently rotated by applying a transverse AC magnetic field. This process allows for the creation of an arbitrary superposition state, with the coefficients spanning the Bloch sphere encoding the qubit information.

A system consisting of two spin-1/2 electrons has four possible spin eigenstates — one antisymmetric singlet state

$$S(0,2) = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle), \quad (1.4)$$

with total angular momentum 0 and three symmetric triplet states (1, 1)

$$T_+ = |\uparrow\uparrow\rangle, \quad (1.5)$$

$$T_0 = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle), \quad (1.6)$$

$$T_- = |\downarrow\downarrow\rangle, \quad (1.7)$$

with the total angular momentum 1. Triplet states are degenerate which can be split by the Zeeman effect following Eq. 1.3. However, S and T_0 states remain degenerate. When

the exchange coupling J between two electrons, confined in two quantum dots, is turned ON, it lowers the energy of spin-singlet state S_0 by J . This singlet-triplet splitting caused by the exchange interaction is described by the Heisenberg exchange Hamiltonian having the form

$$H = J \vec{S}_i \cdot \vec{S}_j, \quad (1.8)$$

where $\vec{S}_i$ is the spin-1/2 operator of an electron confined in the i^{th} dot. By controlling the exchange coupling, it is possible to perform controlled rotations (*CROT*) of the spin state in the $S - T_0$ axis of the Bloch sphere [4]. This is achieved by turning ON the exchange coupling J , which is facilitated by lowering the barrier height between the dots, allowing for interdot tunnel coupling t_c . Thus, J has the form $4t_c^2/u$, where u is the charging energy of a dot.

1.2.3. GATE-DEFINED QUANTUM DOTS

Quantum dots are electrostatically formed in a two-dimensional electron system (2DEG), which is created in a semiconductor heterostructure such as GaAs/AlGaAs. The AlGaAs have a larger band gap, forming a step-like profile in the conduction band minimum. By n-doping the stack with Si, the potential profile is bent, and a single band of electrons is accumulated at the GaAs/AlGaAs interface as shown in Fig. 1.5(a). The triangular-like potential profile restricts the electron movement along the growth direction of the heterostructure, whereas allowed in the other two directions. By applying voltages to gate electrodes deposited on top of the heterostructure, the electrostatic potential of the 2DEG is modulated, leading to the depletion of certain regions and the formation of isolated regions with few electrons, as shown in Fig. 1.5(c). The tight 2D confinement leads to discrete energy states, similar to a quantum dot spectrum.

The GaAs/AlGaAs heterostructure was the first platform to demonstrate the initialization, manipulation, and read-out of a single electron in one quantum dot [5] and two-qubit gates in two quantum dots [6]. The 2DEGs formed at the GaAs/Al_{0.3}Ga_{0.7}As has high electron mobilities of $10^7 \text{ cm}^2/\text{Vs}$ [7] due to their nearly equal lattice constant ($\approx 0.565 \text{ nm}$). GaAs has a smaller effective mass $m_e = 0.067m_0$ compared to Si and Ge which are also potential candidates for spin qubits. This smaller effective mass leads to large level spacings and allows for large quantum dots with a 100nm dot pitch—the distance between the centers of two dots. This enhances the gate tunability of GaAs quantum dots, making them a preferred choice for early spin qubit experiments. A 1D array of four quantum dots [8] and 2x2 quantum dot array (as shown in Fig. 1.5(d)) [9], have also been demonstrated.

Group IV elements such as Si and Ge are attractive candidates for spin qubit devices, due to their ability to reduce spin decoherence caused by hyperfine interaction with the nuclear spins abundant in the GaAs substrate [10]. Isotopic enrichment of natural $^{\text{nat}}\text{Si}$ results in nuclear-spin-free substrate with 99.924% ^{28}Si [11]. This has led to significant improvements in spin coherence time, with devices such as $^{28}\text{Si}/\text{SiGe}$ showing two orders of magnitude increase in spin coherence time compared to GaAs [12]. Another advantage of Si-based spin qubit device is their ability to be mass-produced using advanced semiconductor device manufacturing. The Si/SiO₂, as shown in Fig. 1.5(b,e) is another promising platform for spin qubit devices [13, 14].

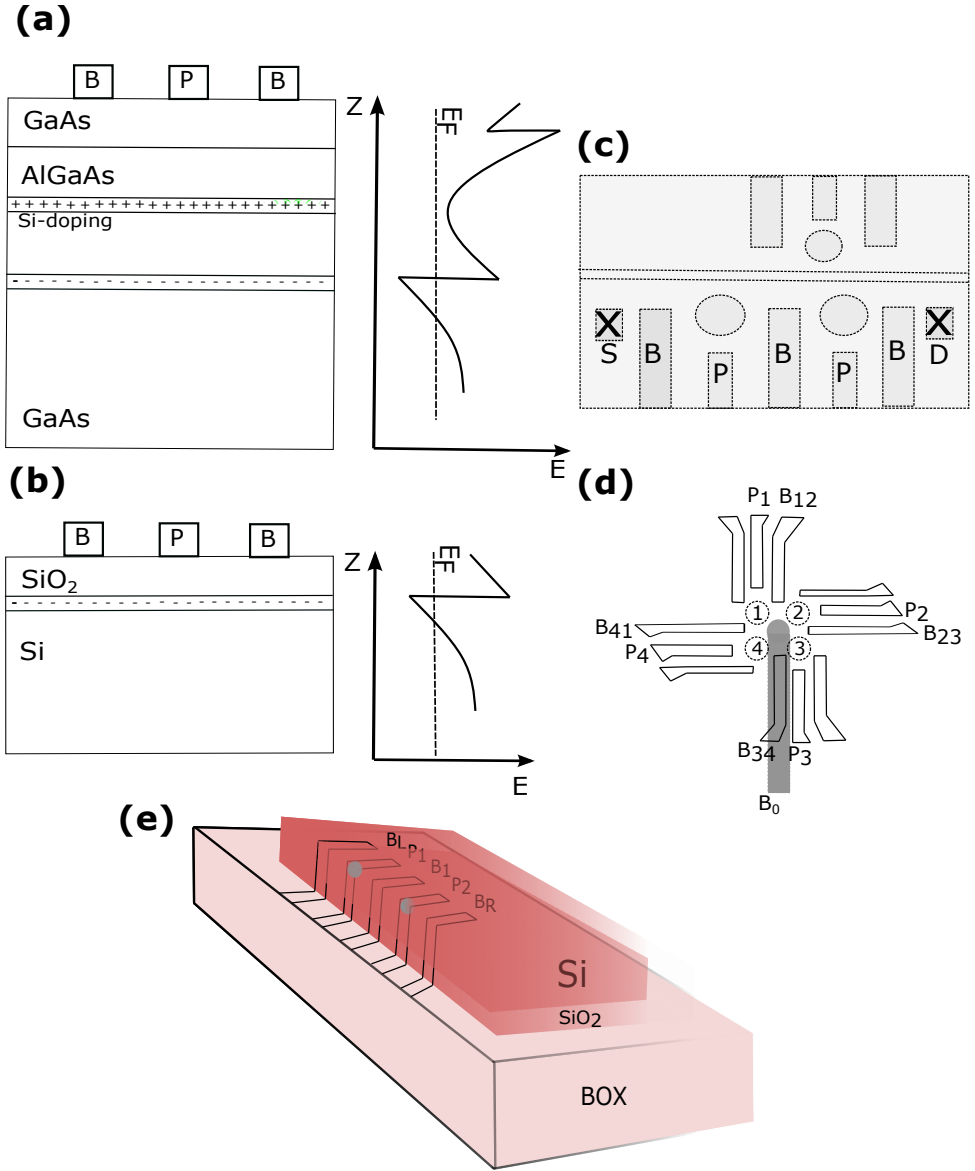


Figure 1.5: Spin qubit device stack. (a) and (b) show the side views of GaAs/AlGaAs and Si heterostructure, respectively, with their energy level diagram along the growth direction shown on the right. In both cases, the energy level falls below the Fermi energy (E_F) across the quantum well, leading to charge accumulation in the quantum well. The top gates shown are operated in depletion mode in the GaAs/AlGaAs heterostructure, whereas they are operated in accumulation mode in the Si heterostructure due to the absence of a dopant layer. (c) Top view of the GaAs heterostructure with depletion gates and charge reservoirs. Two quantum dots and one sensing dot are represented by circles. (d) 2x2 quantum dot array with a central barrier gate (e) Si spin qubit device with non-planar gates forming two quantum dots at the edge of Si/SiO₂ interface.

Disorder makes device tuning extremely difficult. Disorder in the potential landscape of a 2DEG can lead to large device-to-device variability. In modulation-doped GaAs devices, disorder is induced by unionized dopant charges [15]. In contrast, Si-based devices operate in accumulation mode, where charges are electrostatically accumulated in the Si quantum well instead of adding dopant atoms [16]. This has led to high mobility 2DEG in Si/SiGe [17] and Si/SiO₂ [18], indicating low disorder [15]. However, undoped heterostructures are affected by charged defects at the semiconductor-oxide interface [17, 18], as shown in Fig. 1.6. As long as the 2DEG is formed far enough from the interface, the effects of charged defects remain low. However, to ensure a sharp confinement profile for quantum dots, the 2DEG must remain close enough to the gate electrodes. In Si devices, this is likely the case due to the larger effective mass $m_e = 0.19m_0$ compared to GaAs, which demand smaller quantum dots. To achieve tight confinement for smaller quantum dots, the gate electrodes are made smaller and closer, overlapping in a specific fashion [19, 20].

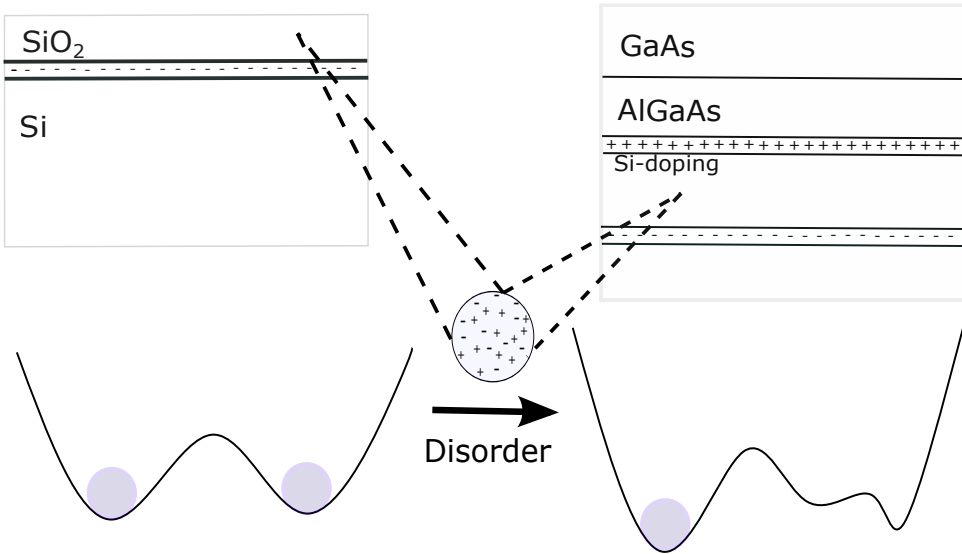


Figure 1.6: Disorder in spin qubit device stack. Positive and negatively charged defects are randomly distributed either in oxide in Si or semiconductor in GaAs heterostructure. As a result, the uniform parabolic confinement profile becomes highly non-uniform creating centers for parasitic dots or shallow centers that are less likely to confine a dot.

1.3. MAJORANA QUBITS

Majorana zero modes (MZM) are non-Abelian anyons that appear as quasiparticle excitations in condensed matter systems. These quasiparticles are formed when indistinguishable particles, such as fermions or bosons, are confined in a two-dimensional system and have excitations above their ground state. In contrast to Abelian anyons, which are characterized by a property known as Abelian statistics, MZMs are non-Abelian anyons that exhibit a different property. Specifically, when the positions of MZMs are

adiabatically exchanged, their initial state is left unchanged up to an arbitrary phase θ ,

$$\psi(r_1, r_2) = e^{i\theta} \psi(r_2, r_1), \quad (1.9)$$

where θ is 0 and π for bosons and fermions respectively. In a system with a degenerate ground state consisting of many localized quasiparticles, the exchange operation can be represented by a unitary matrix U

$$\psi_a \mapsto U_{ab} \psi_b, \quad (1.10)$$

which defines the unitary transformation within the subspace of degenerate ground states. Since matrix multiplication does not commute, the order of exchange operations or unitary transformations matters. This non-Abelian exchange statistics exhibited by Majorana zero modes make them less susceptible to errors from local perturbations, which can occur due to the inherent noise present in quantum systems [21, 22].

Two platforms have been extensively studied to experimentally realize MZM. First, 2DEG in a GaAs/AlGaAs heterostructure with strong perpendicular magnetic fields [23]. This system has been shown to exhibit the $\nu=5/2$ fractional quantum Hall effect (FQHE), in which charge- $e/4$ quasiparticles exist those hypothesized to be MZMs. Second, vortices in a chiral p-wave superconductor. In this system, a bound state at zero energy is predicted, which contains MZMs [24]. p-wave superconductors have spin-triplet pairing, which is a requirement for the existence of MZMs. However, experimental realization of p-wave superconductors has not been achieved yet. As a result, experimentally realizing MZMs is a significant challenge.

1.3.1. 1D KITAEV CHAIN

In 2001, Kitaev proposed a toy model that could potentially lead to the formation of unpaired MZMs at the edges of a one-dimensional chain of fermions. The toy model has the form

$$H = \sum_i^N -\mu \left(c_i^\dagger c_i - \frac{1}{2} \right) - t \left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i \right) + \Delta c_i c_{i+1} + \Delta^* c_{i+1}^\dagger c_i^\dagger, \quad (1.11)$$

where Δ is the p-wave superconducting pairing, where N is the number of sites, μ is the chemical potential, t is the hopping amplitude, $c^\dagger$, and c are the fermion creation and annihilation operators. Here, $\Delta = |\Delta|e^{i\varphi}$ with φ being the superconducting phase. Each site has two Majorana operators γ_{2i-1} and γ_{2i} which anti-commute

$$\gamma_a \gamma_b + \gamma_b \gamma_a = 2\delta_{ab}, \quad (1.12)$$

which is similar to the anti-commutation relation of Fermion operators, but differs from the fact that $\gamma_a^2 = 1$. This follows from the particle-antiparticle equivalence of a Majorana quasiparticle as proposed by Ettore Majorana in 1937 [25]

$$\gamma^\dagger = \gamma, \quad (1.13)$$

where $\gamma^\dagger$ and γ are the Majorana creation and annihilation operators. Therefore, every fermion operator can be expressed as a pair of Majorana operators as

$$c^\dagger = \frac{1}{2} (\gamma_{2i-1} + i\gamma_{2i}), \quad (1.14)$$

$$c = \frac{1}{2} (\gamma_{2i-1} - i\gamma_{2i}). \quad (1.15)$$

To exploit the non-Abelian property of MZM for topological quantum computation, paired MZMs in the Kitaev chain need to be unpaired. With that goal, Eq. 1.11 is rewritten in terms of Majorana operators

$$\gamma_{2i-1} = e^{\frac{i\varphi}{2}} c_n + e^{\frac{-i\varphi}{2}} c_n^\dagger, \quad (1.16)$$

$$\gamma_{2i} = -ie^{\frac{i\varphi}{2}} c_n + ie^{\frac{-i\varphi}{2}} c_n^\dagger, \quad (1.17)$$

as

$$H = \frac{i}{2} \sum_{i=1}^N -\mu \gamma_{2i-1} \gamma_{2i} + (t + |\Delta|) \gamma_{2i} \gamma_{2i+1} + (-t + |\Delta|) \gamma_{2i-2} \gamma_{2i+2}. \quad (1.18)$$

There are two possible cases depending on the choice of parameters. 1. When $|\Delta| = t = 0$

$$\text{a) } |\Delta| = t = 0, \mu < 0$$



$$\text{b) } |\Delta| = t > 0, \mu = 0$$

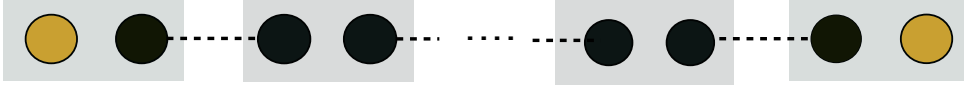


Figure 1.7: (a) One-dimensional chain of fermionic modes a) paired and b) unpaired at the corners which are Majorana zero modes.

and $\mu < 0$, Eq. 1.11 becomes

$$H = \frac{i}{2} \sum_{i=1}^N -\mu \gamma_{2i-1} \gamma_{2i}, \quad (1.19)$$

where all the MZM remain paired. In terms of Fermion operators, Eq. 1.19 becomes

$$H = -\mu \sum_{i=1}^N \left(c^\dagger c_n - \frac{1}{2} \right). \quad (1.20)$$

2. When $|\Delta| = t > 0$ and $\mu = 0$,

$$H = it \sum_{i=1}^{N-1} \gamma_i \gamma_{i+1}, \quad (1.21)$$

two Majorana zero modes at each corner of the chain become unpaired. Ignoring the unpaired Majorana operators and rewriting the Fermion operators

$$\tilde{c}_n = \frac{1}{2} (\gamma_{2i} + i\gamma_{2i+1}), \quad (1.22)$$

$$\tilde{c}_n^\dagger = \frac{1}{2} (\gamma_{2i} - i\gamma_{2i+1}), \quad (1.23)$$

leads to

$$H = 2t \sum_i^{N-1} \left(\tilde{c}_n^\dagger \tilde{c}_n - \frac{1}{2} \right), \quad (1.24)$$

in which the prefactor $2t$ corresponds to the gap in the bulk of the chain.

1.3.2. FAULT TOLERANCE

In Kitaev's toy model, a quantum bit of information is non-locally stored in an unpaired MZM. This unpaired MZM combines into a single fermion, which can either be occupied in the state $|1\rangle$ or unoccupied in the state $|0\rangle$. This defines a two-level system for encoding a qubit *non-locally*. The key advantage of this approach is that a complex fermion operator can be split into two real Majorana operators i.e. $c = \gamma_1 + i\gamma_2$. By separately storing the real and imaginary terms of a qubit in an unpaired MZM, dephasing of a qubit is avoided [26]. This means that the qubit remains coherent and can be manipulated without losing its quantum information. Moreover, the fermion parity which is an observable in measurements that denotes whether a system has an even or odd number of fermions is given by

$$c^\dagger c = \frac{1}{2} (1 + i\gamma_1\gamma_2). \quad (1.25)$$

It signifies that parity can be measured only by *jointly* measuring the two unpaired MZMs because one of them alone does not contain any information. To ensure that the unpaired

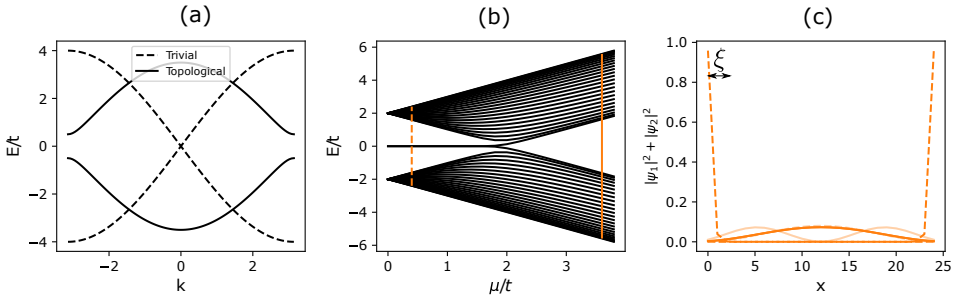


Figure 1.8: (a) The bandstructure of an infinite Kitaev chain with $\mu = -2t$ and $\mu = 1.5t$ shows the emergence of trivial and topological zero-energy modes, respectively. A topological gap is present at $k = \pi$. (b) The energy spectrum of a finite Kitaev chain with $L=25$ nodes exhibits a two-fold degenerate ground state at $E = 0$, which is topologically protected from decoherence sources by particle-hole symmetry as evident from the states below and above the zero energy. (c) Wavefunctions corresponding to the ground and first excited states are depicted, with μ in the topological regime (dashed orange line in (b)) and trivial regime (solid orange line in (b)). ξ is superconducting coherence length.

MZMs do not couple into an excited state and lift the degeneracy of the ground state, the distance between them must be sufficiently large. As mentioned before, a non-Abelian exchange operation of MZMs unitarily transforms a subspace of degenerate ground states. To achieve this, a pair of MZMs must be localized at fixed positions and remain separated by a distance, as shown in Fig. 1.8(c). Furthermore, the ground state degeneracy must vanish exponentially as the distance between the MZMs is decreased [21]. It is only possible [22] if the commutation relation between the Majorana operator and Hamiltonian H is

$$[H, \gamma] \sim e^{-l/\xi}, \quad (1.26)$$

where l is the distance between unpaired MZM and ξ is the superconducting coherence length.

When the degenerate ground state of the unpaired MZM couples to an excited state from the environment, it can result in a mixed state that is an arbitrary superposition of the ground state and an excited state. In this scenario, recovering the state of quantum information by measuring would be impossible even with error-correcting protocols. However, MZMs localized in the midgap of a superconductor are naturally protected from decoherence due to their particle-hole symmetric property. Particle-hole symmetry ensures that for every particle at positive energy $+E$, there is an equivalent anti-particle or *hole* at negative energy $-E$ and the energy spectrum is symmetric around $E = 0$, as shown in Fig. 1.8(b). Protection by particle-hole symmetry ensures that the quantum information encoded in these MZMs remains intact, making them a promising platform for quantum computing applications. To understand the significance of particle-hole symmetry in the fault-tolerant nature of MZMs, we can rewrite Eq. 1.11 as

$$H = \frac{1}{2} C^\dagger H_{BDG} C, \quad (1.27)$$

where C is a column vector that stacks all the creation operators beneath the annihilation operators as $C = (c_1, c_2, \dots, c_n, c_1^\dagger, c_2^\dagger, \dots, c_n^\dagger)^T$. H_{BDG} is a matrix known as Bogoliubov-de Gennes Hamiltonian and has the form

$$H_{BDG} = \begin{pmatrix} H & \Delta \\ \Delta^* & -H^* \end{pmatrix}, \quad (1.28)$$

where the superconducting pairing term Δ is an antisymmetric matrix. H_{BDG} acts on creation operators followed by annihilation operators of particles. As creation operators of particles can be related to annihilation operators of holes, H_{BDG} has particle-hole symmetry. It is represented by an anti-unitary operator $\mathcal{P} = \tau_x \mathcal{K}$ where $\mathcal{K}$ is the complex-conjugate and τ_x is the Pauli-matrix that acts on particle and hole blocks in H_{BDG} . $\mathcal{P}$ anti-commutes with H_{BDG}

$$\mathcal{P} H_{BDG} \mathcal{P}^{-1} = -H_{BDG}, \quad (1.29)$$

where the minus sign due to the anti-commutation property leads to a state at $-E$ for every state at $+E$. Therefore, one of the unpaired Majorana modes cannot move away from $E = 0$. The only way to excite them to a higher energy state is to bring them closer together. This means that as long as the chemical potential does not exceed the bulk gap (i.e. $\mu \lesssim 2t$), the unpaired MZMs remain protected from local perturbations by

particle-hole symmetry, as evident from Fig. 1.8(b). This also implies that precise tuning of chemical potential is not necessary to create unpaired MZMs, and any small local perturbations to μ will not destroy them.

1.3.3. TOPOLOGY IN THE KITAEV CHAIN

Protection of MZMs in the Kitaev chain by a finite bulk gap can be understood through the topological classification of its bulk Hamiltonian. If a transformation exists that continuously deforms a gapped Hamiltonian $H1$ to $H2$ without ever closing the gap and preserves all symmetries, then $H1$ and $H2$ are said to be topologically equivalent. Otherwise, they are considered to be in different topological phases. One way to classify the bulk Hamiltonians based on their topological equivalence is to compute their topological invariant. For a 1D Kitaev chain with particle-hole symmetry, the topological invariant is defined by the sign of the Pfaffian of the Hamiltonian

$$Q = \text{sgn} \text{Pf}(iH), \quad (1.30)$$

which can take only two values ± 1 , and is called $\mathbb{Z}_2$ invariant. In a superconductor with particle-hole symmetry, a pair of electron and hole levels at $\pm E$ is considered to be in a single superposition state and is referred to as a *Bogoliubov quasiparticle*. When those levels cross zero energy point, it means that the gap closes, and the fermion parity changes from even to odd or vice-versa. An odd number of levels crossing $E = 0$ indicates that a Bogoliubov quasiparticle can either be added or removed.

The Pfaffian is computed by considering an infinitely long Kitaev chain and rewriting the Hamiltonian in Eq. 1.18 in the momentum (k) space $H(k)$ using Bloch representation. Due to the particle-hole symmetry in a superconductor, H can be defined as an anti-symmetric matrix, which ensures that the Pfaffian is always defined. The symmetry also causes both electron and hole levels to cross zero energy in pairs at finite momentum in the Brillouin zone. Hence, Pfaffian does not change and the topological invariant remains the same. However, at $k = 0$ and $k = \pi$, the gap closes, indicating the Bogoliubov quasiparticle excitation and a switch in fermion parity. As a result, the Pfaffian changes at those points, and the topological invariant is computed by multiplying them

$$Q = \text{sgn}(\text{Pf}[iH(0)]\text{Pf}[iH(\pi)]). \quad (1.31)$$

$Q = -1$ means the chain has MZM and it is in *topologically non-trivial* phase, otherwise in *trivial* phase.

1.3.4. EXPERIMENTAL REALIZATION

To experimentally realize unpaired Majorana zero modes, it is necessary to have spinless fermions. Kitaev chain model considers only a single spin band, assuming the existence of a p-wave superconductor with spin-triplet pairing. However, this type of pairing is fragile to disorder and easily destroyed. To address this challenge, researchers proposed in 2008 inducing effective p-wave superconductivity through spin-orbit coupling in a topological insulator proximitized by a conventional s-wave superconductor [27]. Topological insulators, characterized by an insulating bulk and a 2D conducting surface with massless Dirac Fermion, have been identified as a promising platform for this purpose [28]. By

depositing an s-wave superconductor on the surface of a topological insulator, the proximity effect occurs, inducing a gap through Cooper pair tunneling. Applying a magnetic field closes the gap locally, binding Majorana states to superconductor vortices at zero energy. Alternatively, the 3D topological insulator can be replaced with a semiconductor film exhibiting strong spin-orbit coupling [29].

A well-studied platform for realizing Majorana zero modes is a semiconductor nanowire with strong spin-orbit coupling that is proximitized by a conventional s-wave superconductor in the presence of a magnetic field [30]. This hybrid device, which combines multiple elements to capture the complex interactions between the various components, is described by an effective Hamiltonian

$$H = \left(\frac{\hbar^2 k^2}{2m^*} - \mu \right) \sigma_0 \tau_z + \Delta \sigma_0 \tau_x + E_z \sigma_x \tau_0 - \alpha k \sigma_y \tau_z, \quad (1.32)$$

where σ_0 and τ_0 are identity matrices, σ_i and τ_i with $i = x, y, z$ are the Pauli matrices acting on the spin and particle-hole space respectively. μ is the chemical potential in the nanowire. The chemical potential in a semiconductor can be controlled with gate voltages. By adjusting the chemical potential to be near the band bottom, only the lowest energy band is occupied. As a result, the first term in Eq. 1.32 corresponds to two parabolic bands, as illustrated in Fig. 1.9(a).

The second term, $\Delta \tau_x$, introduces particle-hole symmetry by coupling the electron and hole bands, forming a gap as shown in Fig. 1.9(b). However, the system remains in a topologically trivial phase due to the presence of time-reversal symmetry. This asymmetry causes the energy bands to be spin-degenerate, a phenomenon known as Kramer's degeneracy, which prevents the system from exhibiting topological properties.

When applying a magnetic field B , it lifts the Kramer's degeneracy by Zeeman coupling to the spin, splitting the spin-degenerate bands as shown in Fig. 1.9(c). The energy splitting is given by $E_Z = \frac{1}{2} g \mu_B B$, where g is the Landé g-factor and μ_B is the Bohr magneton. However, the spin of a state along the x-direction is conserved by the Zeeman effect, which means that Majoranas would need to have a definite spin, which is not possible. As the magnetic field is increased, the two bands approach each other, but they do not couple because they have opposite spin and therefore do not induce a gap, as shown in Fig. 1.9(c). To break spin conservation, it is necessary to couple an electron's motion to its spin under an external electric field. When an electron moves parallel to the nanowire under an external electric field $\vec{E}$, it generates a perpendicular magnetic field $\vec{B}_{SO} \propto \vec{k} \times \vec{E}$, which breaks the spin conservation. This leads to an effective term $-\alpha k \sigma_y$ with α , the Rashba spin-orbit interaction (SOI) strength, that depends on the electric field strength $|E|$ and the semiconductor material. Here, k is the momentum along the nanowire axis, $\vec{k} = (k, 0, 0)$. The spin-orbit interaction causes the spin-degenerate bands to split, effectively pushing them away from each other along the $+k$ and $-k$ directions. This couples two spin bands and in the presence of a magnetic field, a gap opens in the spectrum, as shown in Fig. 1.9(d). At $k = 0$, Eq. 1.32 becomes

$$H(k=0) = -\mu \sigma_0 \tau_z + \Delta \sigma_0 \tau_x + E_z \sigma_x \tau_0, \quad (1.33)$$

which can be diagonalized to obtain the eigenvalues

$$E(k=0) = \pm E_Z \pm \sqrt{\mu^2 + \Delta^2}. \quad (1.34)$$

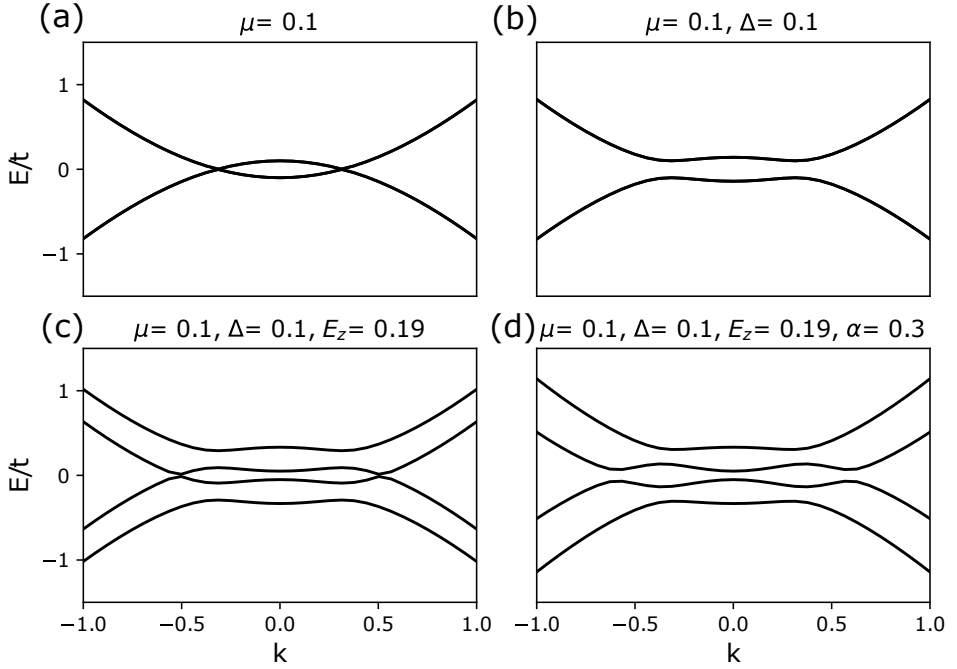


Figure 1.9: Bandstructure of infinite nanowire shown by adding ingredients essential to form MZM one at a time. (a) Two parabolic bands are formed by tuning the chemical potential μ of the semiconductor nanowire. (b) Gap opening between spin-degenerate bands as a result of particle-hole symmetry. (c) Adding an external magnetic field induces the Zeeman effect and lifts the spin-degeneracy with still no gap at $E=0$. (d) Spin-orbit interaction induced by external electric field induces a gap at $E = 0$.

For $E_z = \sqrt{\mu^2 + \Delta^2}$, the gap closes and the system enters topological phase transition. When $E_z > \sqrt{\mu^2 + \Delta^2}$, the gap reopens again in the presence of spin-orbit interaction. This leaves the system in a topologically non-trivial phase where Majoranas form at zero energy ($E = 0$).

1.3.5. TOPOLOGICAL QUANTUM COMPUTATION

Our motivation for studying Majorana zero modes comes from the fact that they are non-Abelian anyons. Braiding them results in non-trivial rotations within the single-qubit Bloch sphere, which defines a basis for a topologically protected qubit. To demonstrate the non-abelian exchange statistics of MZM, we require a network of MZMs.

In the previous subsection, we studied engineered 1D semiconductor-superconductor nanowires as a platform to experimentally realize Majorana zero modes. We found that by tuning the chemical potential μ , we can open or close the gap, which determines whether the system is in a topologically non-trivial or trivial phase. When $\mu < \mu_c = \sqrt{E_z^2 - \Delta^2}$, the spectrum has a gap, and the system is in a topologically non-trivial phase. If $\mu = \mu_c$, the gap closes, and MZMs do not form. In a semiconductor, μ can be tuned by tuning the gate voltages. Locally tuning μ of a long nanowire using local gates, it is possible to create

a network of N Majoranas [31].

In one dimension, braiding is not well-defined, as it is difficult to ensure that two Majoranas remain well-separated by a distance l during braiding. However, when exchanging their positions along a nanowire, the Majoranas must come closer to each other, allowing them to fuse into a quasiparticle that excites to a state above the gap. Therefore, we need an additional dimension to facilitate the exchange operation without causing the Majoranas to fuse.

Alicea et.al. [31] proposed a solution to the braiding problem by connecting an ancillary nanowire perpendicularly to the main nanowire, forming a T-junction. One of the Majoranas, γ_1 , temporarily resides in the ancillary nanowire, while the other Majorana, γ_2 , travels through the main nanowire and occupies the position held by γ_1 . This allows any two Majoranas in a network of T-junctions to be exchanged in a clockwise or anti-clockwise manner, effectively braiding them without causing them to fuse.

To gain a deeper understanding of the non-Abelian exchange statistics of MZMs, let's consider the following scenario. Assume that the nanowire is locally driven into the topological phase, by which one Majorana forms at a domain wall with a T-junction in between. In this scenario, $2N$ Majorana modes are formed, which can be considered as N fermionic modes. Each of these fermionic modes can be either occupied by an electron $|1\rangle$ or unoccupied $|0\rangle$. This leads to a *ground state manifold* with 2^N -fold degenerate ground states. This manifold is separated from the finite energy continuum states by a gap Δ .

Spatially exchanging two neighboring Majoranas leaves the final state within the ground state manifold. This means as long as the whole process is adiabatic, the system remains gapped and the total fermion parity is preserved. The fermion parity operator is defined as

$$P_n \equiv 1 - 2c_n c_n^\dagger = 1 - \gamma_{2n-1} \gamma_{2n}, \quad (1.35)$$

and the total fermion parity of the system is determined by multiplying each of them (for every pair of Majorana)

$$P_{tot} = P_1 \cdot P_2 \cdots P_N = i^N \gamma_1 \gamma_2 \cdots \gamma_{2N}. \quad (1.36)$$

Finally, the unitary transformation which connects initial and final states post-exchange operation commutes with the total fermion parity, $[U, P_{tot}] = 0$. U depends only on the product of the pair of Majorana operators involved in the exchange, $i\gamma_n \gamma_m$, which is a Hermitian operator. Therefore, U in general, has the form

$$U \equiv \exp(\beta \gamma_n \gamma_m) = \cos(\beta) + \gamma_n \gamma_m \sin(\beta), \quad (1.37)$$

with the equality obtained using the relation $(\gamma_n \gamma_m)^2 = 1$. Here, β is a real coefficient that can be determined by taking the time evolution of the Majorana operators in the Heisenberg picture

$$\gamma_n \rightarrow U \gamma_n U^\dagger, \quad (1.38)$$

$$\gamma_m \rightarrow U \gamma_m U^\dagger. \quad (1.39)$$

Applying the relation from Eq. 1.37, γ_n and γ_m becomes

$$\gamma_n \rightarrow \gamma_n \cos(2\beta) - \gamma_m \sin(2\beta), \quad (1.40)$$

$$\gamma_m \rightarrow \gamma_m \cos(2\beta) + \gamma_n \sin(2\beta). \quad (1.41)$$

The exchange, $\gamma_n \rightarrow \gamma_m$ and $\gamma_m \rightarrow \gamma_n$, sets the condition $\beta = \pm \frac{\pi}{4}$, where the sign distinguishes clockwise from the anti-clockwise operation. Thus, the unitary transformation takes the form

$$U = \exp\left(\pm \frac{\pi}{4} \gamma_n \gamma_m\right) = \frac{1}{\sqrt{2}} (1 \pm \gamma_n \gamma_m). \quad (1.42)$$

To understand the role of unitary transformation, we consider four Majoranas $\gamma_1, \gamma_2, \gamma_3$, and γ_4 . Two of these operators combine into a single fermionic state. Denoting their occupation by either $|0\rangle$ or $|1\rangle$, generates 4-fold degenerate ground state with the eigenstates $|00\rangle, |01\rangle, |10\rangle$, and $|11\rangle$. Starting from the eigenstate $|00\rangle$ and exchanging two neighboring Majoranas, say γ_2 and γ_3 , through $U_{23} = \frac{1}{\sqrt{2}} (1 \pm \gamma_2 \gamma_3)$ as follows

$$|00\rangle \rightarrow U_{23} |00\rangle = \frac{1}{\sqrt{2}} (|00\rangle - i |11\rangle), \quad (1.43)$$

results in a superposition of two eigenstates¹. In contrast to the trivial phase changes observed in bosons and fermions, the non-trivial phase change resulting from exchanging MZMs demonstrates their non-Abelian anyonic nature. This process known as braiding, involves the exchange of two non-Abelian anyons. Regardless of the specific braiding operation performed, the initial and final states are linked by an operator, specifically $\exp(\pm \frac{\pi}{4} \gamma_n \gamma_m)$. Moreover, quantum information is non-locally stored in MZMs, which is also topologically protected. This property makes braiding MZMs a promising platform for fault-tolerant quantum computation. Implementing an experimentally feasible Majorana braiding platform is a complex challenge. To avoid Majorana collisions during exchange, the platform requires at least a two-dimensional degree of freedom. A promising approach is the use of nanowires with a T-junction, which offers a quasi-2D environment for Majorana exchange. Alternatively, Sau et.al. [32] proposed another braiding platform based on nanowires tunnel-coupled in a trijunction configuration. Three proximitized nanowires, each tuned to the topological phase, host corner Majorana zero modes. The trijunction is comprised of three non-proximitized nanowires, as shown in Fig. 1.10(b). Nanowires in trijunction form a gate-controlled tunnel barrier between the adjacent Majoranas. Notably, any two Majoranas remain paired throughout the braiding process. Majoranas are exchanged by simultaneously decreasing the tunneling amplitude of a fermionic mode and increasing the tunneling between adjacent unpaired Majoranas. The time evolution of this process is described by the Hamiltonian [32]

$$H(t) = [\zeta_{12} \alpha(t) \gamma_1 \gamma_2 + \zeta_{23} (1 - \alpha(t)) \gamma_2 \gamma_3], \quad (1.44)$$

where ζ_{12} and ζ_{23} are the tunneling amplitudes across the nanowire that couples the Majoranas 1 and 2, and 2 and 3 respectively. Here, $\alpha(t)$ is changed adiabatically from 0 ($t = 0$) to 1 ($t = T$).

¹It is the case regardless of the exact form of the matrix U_{23} given that it is a unitary transformation.

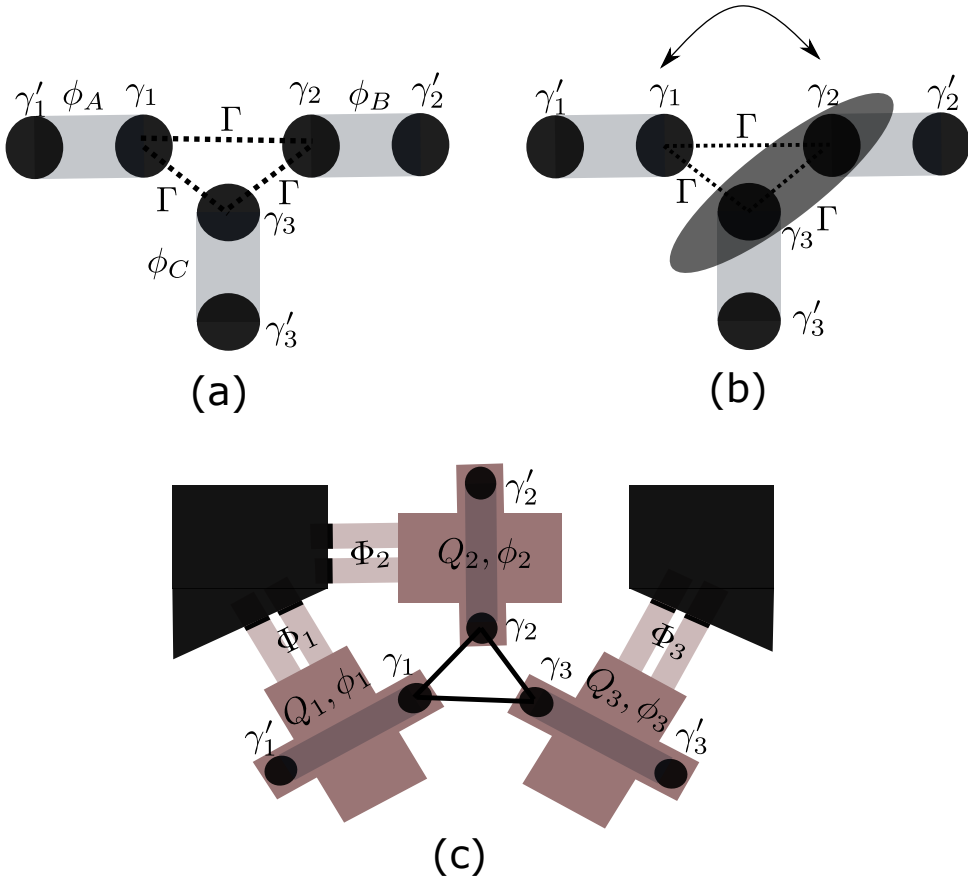


Figure 1.10: Braiding proposals for topological quantum computation. (a) Alicea et.al. [31] suggested a T-junction consisting of three nanowires that have been driven into the topological regime with a superconducting phase Φ . Each nanowire hosts two MZMs at its corner. MZMs near the junction in the middle are tunnel-coupled with amplitude Γ , which can be controlled by external gate voltages. (b) Sau et.al. [32] proposed a similar T-junction, where any two MZMs among the three closest to the junction remain tunnel-coupled (denoted by black semi-transparent ellipse around two MZMs) throughout the braiding, resulting in one higher-energy fermionic mode and one MZM. This allows for the positional exchange of two Majoranas. (c) B. van Heck et.al. [33] proposed a trijunction with Majorana nanowires within a Cooper box. MZMs can be coupled via Coulomb interactions through the magnetic flux Φ enclosed by the split Josephson junction connected to the bulk superconductor (black polygon).

Instead of tunnel coupling, B. van Heck et.al. [33] used Coulomb interactions to couple distant Majoranas. They designed a trijunction configuration comprising three *Cooper pair boxes*, which are superconducting islands hosting unpaired Majoranas, as depicted in Fig. 1.10(c). These islands are connected to a bulk superconductor, forming a split Josephson junction that encloses magnetic fluxes Φ_1 , Φ_2 , and Φ_3 . Coulomb coupling between unpaired Majoranas in three nanowires is controlled by these fluxes and can be made exponentially small. Three Majoranas adjacent to the trijunction are tunnel-

coupled, effectively resulting in a single fermionic excitation and one MZM. When the coulomb coupling is weaker than the tunnel coupling, the system has four MZMs in the ground state.

1.4. DEVICE MODELING

Our goal is to develop an optimal gate design for spin- and Majorana qubits, which are vulnerable to disorder in their semiconductor device stacks. Disorder can significantly degrade the performance of these qubits, making it crucial that we employ an effective simulation approach. To achieve this, we simulate various gate designs for both types of qubits in the presence of disorder. When simulating gate designs under disordered conditions, selecting the optimal modeling approach is vital. The chosen approach must provide accurate and reliable results while minimizing computational costs. In our research, we have explored capacitive circuit models and Kitaev's chain in the context of quantum dots and nanowires. Both are minimal models that rely on simplified descriptions of the system, offering quick qualitative results that are easier to interpret. However, to accurately study the impact of disorder on qubit characteristics, we require models that can accurately describe both the electronic structure of semiconductors and electrostatic phenomena. These tasks exceed the capabilities of minimal models, emphasizing the need for more sophisticated approaches.

On the other hand, there exist approaches that rigorously model electronic properties at an atomic level. For instance, atomistic tight binding methods that account for multiple bands and sp^3d^5 orbitals are used to study deformation potentials in strained semiconductors such as Si and Ge [34]. Strain plays a significant role in spin qubit research as it offers benefits such as lifting valley degeneracy in Si. However, our primary focus lies in electrostatic phenomena rather than strain. While atomistic models are accurate compared to experimental results, they come with a high computational cost that scales cubically with the number of atoms N ($\mathcal{O}(N^3)$). This makes them impractical for large systems. For example, spin- and Majorana-qubit systems featuring 2DEG typically contain 10^7 to 10^8 number of atoms, making it unfeasible to study these systems using atomistic models.

We aim for a middle ground between minimal and atomistic modeling approaches by seeking a method that is tailored to our specific needs. In this context, we use the $\mathbf{k} \cdot \mathbf{p}$ approach to model the 2DEG formed in a semiconductor heterostructure. This semi-empirical method, discussed further in subsection 1.4.1, offers a balance between capturing essential quantum physics and handling large systems with reasonable computational costs. Furthermore, we investigate the relationship between gate voltages and electrostatic potential in the presence of disorder, requiring more rigorous electrostatic approaches than analytical models [35]. We use numerical Poisson solvers to achieve this. In summary, we deliberately chose a semi-empirical approach that incorporates essential details specific to our use cases.

1.4.1. SEMI-EMPIRICAL APPROACHES

This thesis explores the calculation of the low-energy spectrum in semiconductor devices, such as quantum dots and nanowires, which exhibit few-electron states or Majorana

zero modes as illustrated in Fig. 1.11. These states are situated below the Fermi energy (typically set to zero), and we employ the $\mathbf{k} \cdot \mathbf{p}$ approach to compute the desired low-energy spectrum.

Modeling a semiconductor heterostructure typically begins with the continuum Hamiltonian containing the kinetic energy and potential energy of a particle. We have seen such a description for Majorana particles in 1D nanowire in the first term of Eq. 1.32. Typically spin qubits are defined in a 2DEG and recent proposals for Majorana qubits based on 2DEGs [36] look promising. Hence, we limit our discussion of spin- and Majorana devices to the 2D continuum Hamiltonian

$$H_{2D} = -\frac{\hbar^2}{2m_e} \left(\partial_x^2 + \partial_y^2 \right) + U(x, y), \quad (1.45)$$

where m_e is the effective electron mass and U is the position-dependent electrostatic potential in the 2DEG. The kinetic energy of particles is described by the effective mass approximation (EMA). It is relevant for semiconductors because the particles in the close vicinity of the bottom(top) of the conduction(valence)—termed as high-symmetry points in the Brillouin zone contribute most to phenomena such as carrier transport. Such a band is considered to be parabolic in EMA and its curvature defines the effective mass of the confined particles

$$m^* = \hbar^2 \left(\frac{d^2 E(\mathbf{k})}{d\mathbf{k}^2} \right)^{-1}, \quad (1.46)$$

where $E(\mathbf{k})$ is the energy of particles with momentum k . Though EMA is simple and useful, when the influence of higher energy states cannot be ignored, the non-parabolic nature of bands must be considered. In this context, the $\mathbf{k} \cdot \mathbf{p}$ approach is most commonly used to study semiconductors. It defines an effective Hamiltonian for particles confined around the high symmetry points by including the effects of higher energy bands using perturbation theory.

To study the $\mathbf{k} \cdot \mathbf{p}$ theory, let us consider 1D Hamiltonian represented in momentum space

$$H = \frac{\hat{\mathbf{p}}_x^2}{2m_0} + U(x), \quad (1.47)$$

where $\hat{\mathbf{p}}_x$ is the particle momentum and $U(x)$ is a periodic crystal potential. We define the time-independent Schrodinger equation

$$H\psi_n(\mathbf{x}) = E_n\psi_n(\mathbf{x}), \quad (1.48)$$

where n is the discrete band index. Taking advantage of the periodic nature of $U(\mathbf{x})$ and using Bloch's function for the wavefunction $\psi_n(\mathbf{x})$, Eq. 1.48 is formulated as

$$H(\mathbf{k})u_{n,\mathbf{k}}(\mathbf{x}) = E_n(\mathbf{k})u_{n,\mathbf{k}}(\mathbf{x}), \quad (1.49)$$

where $\mathbf{k}$ is the crystal momentum, $u_{n,\mathbf{k}}$ is a Bloch function and $H(\mathbf{k})$ is a $\mathbf{k}$ -dependent Hamiltonian

$$H(\mathbf{k}) = \frac{\hat{\mathbf{p}}_x^2}{2m_0} + \frac{\hbar^2 \mathbf{k}^2}{2m_0} + \frac{\hbar}{m_0} \mathbf{k} \cdot \hat{\mathbf{p}} + U(\mathbf{x}). \quad (1.50)$$

Bands closer to the extremum point $\mathbf{k}_0$ in the Brillouin zone may not be well described by EMA when the influence of bands at higher $\mathbf{k}$ is relevant. In that case, we split the term $H(\mathbf{k})$ in Eq. 1.50 into $H(\mathbf{k}_0)$ and $\mathbf{k}$ dependent term as

$$H(\mathbf{k}) = H(\mathbf{k}_0) + \frac{\hbar^2(\mathbf{k}^2 - \mathbf{k}_0^2)}{2m_0} + \frac{\hbar}{m_0}(\mathbf{k} - \mathbf{k}_0) \cdot \hat{\mathbf{p}}, \quad (1.51)$$

with

$$H(\mathbf{k}_0)u_{n,\mathbf{k}_0}(\mathbf{x}) = E_n(\mathbf{k}_0)u_{n,\mathbf{k}_0}(\mathbf{x}), \quad (1.52)$$

where we assume eigenenergies $E_n(\mathbf{k}_0)$ and eigenvectors $u_{n,\mathbf{k}_0}(\mathbf{x})$ are known. The influence of higher $\mathbf{k}$ bands is integrated through perturbation theory as depicted in Fig. 1.11, which we will discuss in Chapter 2.

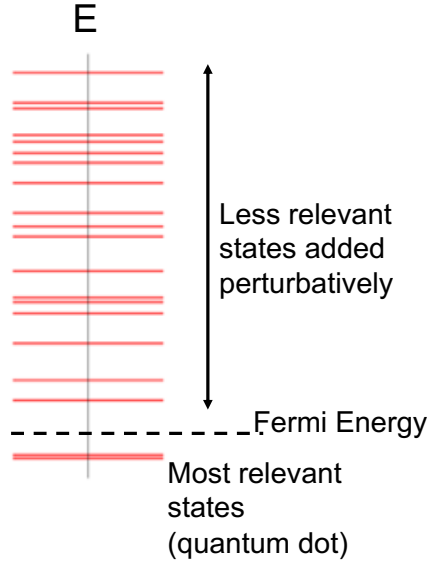


Figure 1.11: Energy states in a quantum dot spectrum those are most- and less relevant to $\mathbf{k} \cdot \mathbf{p}$ -based numerical simulation.

1.4.2. NUMERICAL MODELLING

To accurately model complex gate architectures and multi-layer device stacks, like those depicted in Fig. 1.5, we calculate the electrostatic potential U by numerically solving Poisson's equation

$$\nabla \cdot [\epsilon_r(\mathbf{r}) \nabla U(\mathbf{r})] = -\frac{\rho(\mathbf{r})}{\epsilon_0}, \quad (1.53)$$

where ρ is the charge density including any disorder charges, ϵ_r is the relative permittivity and ϵ_0 is the vacuum permittivity. To investigate the impact of disorder on the system, we introduce random impurities in the gate oxide, as depicted in Fig. 1.6. This type of

disorder is particularly relevant for spin- and Majorana-qubit systems [37, 38]. We employ a numerical electrostatic solver, based on the open-source code from Grenoble [39], to discretize and solve Eq. 1.53 using a finite volume mesh. Notably, the charge density in a 2DEG is typically dependent on the potential U , which means that Eq. 1.53 must be solved self-consistently with the charge density, derived from the wavefunction's probability density

$$\rho(r) = |\psi(r)|^2. \quad (1.54)$$

Solving the electrostatic potential self-consistently with the charge density in a 2DEG is essential for accurate numerical results that match experimental data, unlike relying on pre-defined shapes [35]. However, this approach comes at a significant computational cost due to the iterative diagonalization process, which scales cubically with system size ($\mathcal{O}(N^3)$). Additionally, simulating disorder in semiconductor heterostructures can be computationally intensive, especially when generating multiple configurations to account for randomness. To address these challenges, we employ approximations tailored to our specific use cases, striking a balance between accuracy and computational efficiency. For instance, the highly depleted regime with only a few electrons at the heterointerface significantly reduces the impact of electrostatic potential on charge density distribution. In light of this, we opt out of self-consistent solutions for electrostatic potential and charge density, instead focusing on the more critical aspects of the system, such as disorder effects.

We derive an effective Hamiltonian H_{eff} for the states close to the E_f which are highly relevant as shown in Fig. 1.11. H_{eff} contains energies ϵ_i of states along its diagonal and their couplings t_{ij} in the off-diagonal as

$$H_{eff} = \begin{pmatrix} \epsilon_1 & t_{12} \\ t_{12}^* & \epsilon_2 \end{pmatrix}, \quad (1.55)$$

which can be forced to vary with external electric or magnetic fields. For instance, in Eq. 1.55, the energy of quantum dots ϵ_i and the tunnel couplings t_{ij} vary with the gate voltages. Diagonal and off-diagonal elements of an effective Hamiltonian are the key ingredients to define a cost function for numerical optimization.

To optimize gate geometries for improved performance, it's crucial to pinpoint and refine the critical factors that influence their behavior. Initially, we identified a potential gate design that meets our desired performance criteria through brainstorming and analysis. Next, we use numerical optimization techniques to iteratively adjust key design variables such as gate length (L) and width (W) to maximize performance. Once the gate design is fixed, we fine-tune the gate voltages to ensure the device starts in its expected state and operates within its optimal range. Finally, we incorporate disorder into our simulations to assess the robustness of a specific gate design against measurement uncertainties.

1.5. STRUCTURE OF THIS THESIS

Here is a brief overview of the topics we discussed in the following chapters.

1.5.1. CHAPTER 2: HYBRID KERNEL POLYNOMIAL METHOD

The kernel polynomial method allows to sample overall spectral properties of a quantum system, while sparse diagonalization provides accurate information about a few important states. We present a method combining these two approaches without loss of performance or accuracy. We apply this hybrid kernel polynomial method to improve the computation of thermodynamic quantities and the construction of perturbative effective models, in a regime where neither of the methods is sufficient on its own. To achieve this we develop a perturbative kernel polynomial method to compute arbitrary order series expansions of expectation values. We demonstrate the efficiency of our approach on three examples: the calculation of supercurrent and inductance in a Josephson junction, the interaction of spin qubits defined in a two-dimensional electron gas, and the calculation of the effective band structure in a realistic model of a semiconductor nanowire.

1.5.2. CHAPTER 3: IMPACT OF DISORDER ON THE DISTRIBUTION OF GATE COUPLING STRENGTHS IN A SPIN QUBIT DEVICE

A scalable spin-based quantum processor requires a suitable semiconductor heterostructure and a gate design, with multiple alternatives being investigated. Characterizing such devices experimentally is a demanding task, with the full development cycle taking at least months. While numerical simulations are more time-efficient, their predictive power is limited due to unavoidable disorder and device-to-device variation. We develop a spin-qubit device simulation for determining the distribution of the coupling strengths between the electrostatic gate potentials and the effective device Hamiltonian in the presence of disorder. By comparing our simulation results with the experimental data, we demonstrate that the coupling of the gate voltages to the dot chemical potential and the interdot tunnel coupling match up to disorder-induced variance. To demonstrate the flexibility of our approach, we also analyze an alternative non-planar geometry inspired by FinFET devices.

1.5.3. CHAPTER 4: DESIGN OF A MAJORANA TRIJUNCTION

Braiding of Majorana states demonstrates their non-Abelian exchange statistics. One implementation of braiding requires control of the pairwise couplings between all Majorana states in a trijunction device. To have adiabaticity, a trijunction device requires the desired pair coupling to be sufficiently large and the undesired couplings to vanish. In this work, we design and simulate a trijunction device in a two-dimensional electron gas with a focus on the normal region that connects three Majorana states. We use an optimization approach to find the operational regime of the device in a multi-dimensional voltage space. Using the optimization results, we simulate a braiding experiment by adiabatically coupling different pairs of Majorana states without closing the topological gap. We then evaluate the feasibility of braiding in a trijunction device for different shapes and disorder strengths.

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2

HYBRID KERNEL POLYNOMIAL METHOD

This chapter has been previously published as Muhammad Irfan, Sathish R. Kuppaswamy, Dániel Varjas, Pablo M. Perez-Piskunow, Rafal Skolasinski, Michael Wimmer, and Anton R. Akhmerov, *Hybrid kernel polynomial method*, arXiv:1909.09649. I applied Löwdin perturbation theory to the spin qubit example and wrote that part of the manuscript.

2.1. INTRODUCTION

The behavior of the Fermi sea is governed by both the few partially occupied states near the Fermi level, and the overall effect of the large number of fully occupied states. Therefore, to accurately capture the relevant physics, one needs to combine high resolution information about the former with the integrated contribution of the latter. A similar need to combine integrated information with high resolution arises when constructing effective models using Löwdin partitioning or Schrieffer-Wolff transformation [1–4]. In a computational context, simultaneously satisfying these two requirements is only possible with the full knowledge of the spectrum. Therefore, analyzing a system with size N Hilbert space requires the full cost of $\mathcal{O}(N^3)$ operations of dense linear algebra, prohibiting the exploitation of the sparsity of the Hamiltonian.

Applying a sparse Hamiltonian to a state is cheap. Iterative diagonalization algorithms efficiently utilize this to obtain a small set of eigenenergies and eigenvectors at a low cost [5]. For example, the algorithms implemented in ARPACK [6] combined with a sparse direct linear solver (such as MUMPS [7, 8]) allow to compute several eigenvectors around any interior point of the spectrum. The kernel polynomial method (KPM) [9] also utilizes the sparsity structure, but to obtain limited energy resolution information about the full spectrum. This is possible due to the recursive computation of the Chebyshev decomposition of the Hamiltonian action on a vector.

In this work, we propose a family of algorithms which we call “hybrid KPM” that combine the integral information of KPM with the high precision of diagonalization. The building block of these methods is the amended KPM expansion, where we subtract the contribution of the known part of the spectrum. Hybrid KPM algorithms apply both to the computation of thermodynamic properties at low temperatures, and the construction of effective Hamiltonians restricted to a small subspace. We demonstrate on a set of physical problems that hybrid KPM achieves increased precision at the same computational cost.

We apply and benchmark hybrid KPM by computing supercurrent and Josephson inductance of a long Josephson junction [10–12], where both the contribution of discrete subgap states and the continuum are of the same order. Turning to the effective models, we consider two model systems: the tunneling Hamiltonian of two coupled quantum dots [13], and the band structure of a semiconductor nanowire [14–17]. In both cases, we start from a microscopic Hamiltonian and obtain an accurate effective model, which requires using up to 3rd-order perturbation theory.

2.2. KERNEL POLYNOMIAL METHOD

To compute thermodynamic properties and effective models, one needs to evaluate the action of the Fermi function or Green's function of the Hamiltonian on a state. The kernel polynomial method (KPM) [9] enables an efficient approximation of such functions of operators. We start by rescaling a Hamiltonian $\hat{H}$ such that its spectrum $\{E_k\}$ is bounded to the interval $(-1, 1)$. In general, a function $f(\hat{H}, \lambda)$ of a Hermitian operator $\hat{H}$ and a set of parameters λ can be calculated using the eigendecomposition $\hat{H} = \sum_k E_k |\psi_k\rangle\langle\psi_k|$ as

$$f(\hat{H}, \lambda) \equiv \sum_k f(E_k, \lambda) |\psi_k\rangle\langle\psi_k|, \quad (2.1)$$

where $f(E, \lambda)$ is a scalar function. The expansion in eigenfunctions is computationally expensive since it requires the full diagonalization of $\hat{H}$. This process scales as $\mathcal{O}(N^3)$ with the N size of the Hilbert space.

An alternative approach—KPM—utilizes the expansion of the scalar function $f(E, \lambda)$ in terms of Chebyshev polynomials T_m

$$f(E, \lambda) = \sum_{m=0}^{\infty} \alpha_m(\lambda) T_m(E), \quad (2.2)$$

to build the operator function $f(\hat{H}, \lambda)$ (see Appendix 2.A for expansions of commonly used functions). The Chebyshev polynomials $T_m(x) = \cos(m \arccos x)$ form a complete basis in the interval $(-1, 1)$. They are orthogonal under the inner product

$$\langle f \cdot g \rangle = \int_{-1}^1 \frac{f(x)g(x)}{\pi \sqrt{1-x^2}} dx, \quad (2.3)$$

and satisfy the recursion relation $T_{m+1}(x) = 2xT_m(x) - T_{m-1}(x)$. The Chebyshev coefficients α_m are calculated using the inner product from Eq. (2.3) with variable E

$$\alpha_m(\lambda) = \langle f(E, \lambda) \cdot T_m(E) \rangle, \quad (2.4)$$

and the same coefficients apply to the polynomial expansion of the operator function

$$f(\hat{H}, \lambda) = \sum_{m=0}^{\infty} \alpha_m(\lambda) T_m(\hat{H}). \quad (2.5)$$

We are interested in the action of $f(\hat{H}, \lambda)$ on a set of vectors. In such situations, the expensive part of the computation is to calculate $T_m(\hat{H})|v\rangle$, and once we have done that, the coefficients can be readily computed (in most cases analytically) for any value of the parameters λ .

In practice, the magnitude of the coefficients α_m decays with m and we truncate the series to a finite order M . To stabilize the convergence and avoid Gibbs oscillations, while ensuring positivity, we use either the Jackson or Lorentz kernel [9], which is a set of prefactors $g_{m,M}$ that modify the coefficients to $\tilde{\alpha}_m(\lambda) = g_{m,M} \alpha_m(\lambda)$. The recently developed Chebyshev polynomial Green's function method [18] avoids the need for introducing the kernel by approximating a smoothened Green's function. Because we aim to resolve individual states, we do not expect this technique to be useful in the hybrid setting.

The error of the KPM approximation comes from the function f being replaced by its finite order Chebyshev polynomial approximation:

$$f(\hat{H}, \lambda) \stackrel{\text{KPM}}{\approx} \tilde{f}(\hat{H}, \lambda) \equiv \sum_k \tilde{f}(E_k, \lambda) |\psi_k\rangle \langle \psi_k|, \quad (2.6)$$

with

$$\tilde{f}(E, \lambda) = \sum_{m=0}^M \tilde{\alpha}_m(\lambda) T_m(E). \quad (2.7)$$

This error is small if the function is smooth, or there are no eigenvalues of $\hat{H}$ in regions where it changes fast. The order of the approximation M , together with the choice of the kernel, sets the energy resolution of the approximation, which for the Jackson kernel is inversely proportional to M . The Chebyshev expansion of order M captures features larger than W/M , where W is the full bandwidth of $\hat{H}$ [9].

Hamiltonians and other observables that appear in physical problems are typically sparse matrices where the number of nonzero entries is proportional to the system size N . This allows calculating a sparse matrix–vector product in $\mathcal{O}(N)$ time, much faster than the $\mathcal{O}(N^2)$ scaling of dense matrix–vector products. The recursion relation for Chebyshev polynomials can then be rewritten for the operator function acting on a vector as

$$|v_{m+1}\rangle = 2\hat{H}|v_m\rangle - |v_{m-1}\rangle, \quad (2.8)$$

where $|v_m\rangle = T_m(\hat{H})|v\rangle$. Hence, the Chebyshev expanded action $f(\hat{H}, \lambda)|v\rangle$ up to order M can be computed in $\mathcal{O}(NM)$ time. The computational effort of KPM scales as $\mathcal{O}(NW/\Delta)$ where Δ is the required energy resolution. KPM is most efficient when the desired energy resolution is much coarser than the typical level spacing, that is when $\Delta \gg W/N$, and $M = W/\Delta \ll N$.

The key idea behind hybrid KPM is using a more accurate approximation of $f(\hat{H}, \lambda)$:

$$\begin{aligned} f(\hat{H}, \lambda) \stackrel{\text{hybrid}}{\approx} \tilde{f}(\hat{H}, \lambda) - \sum_{k \in A} \tilde{f}(E_k, \lambda) |\psi_k\rangle \langle \psi_k| \\ + \sum_{k \in A} f(E_k, \lambda) |\psi_k\rangle \langle \psi_k|. \end{aligned} \quad (2.9)$$

Here we combine the KPM approximation of the complete spectrum with the exact contribution of a few states in a small subspace A . To avoid double-counting we subtract the KPM contribution of the exactly known states and add back their exact contribution. Approximation (2.6) has a large error due to states in the energy range where f changes rapidly. Our approach fixes this problem by using a sparse eigensolver to find these states and taking their contribution into account exactly while keeping the energy resolution of KPM low.

2.3. LÖWDIN PERTURBATION THEORY

Quantum systems often have many degrees of freedom, while only a few states (for example the lowest energy ones) are of interest for physical understanding. Perturbative effective models describe such a situation well by constructing a Hamiltonian of the small “interesting” subspace and integrating out the remaining states. After the integration, the effective model includes both a shift in the energy of the eigenstates and additional coupling terms mixing various eigenstates.

We use the Löwdin partitioning approach [1, 3, 4, 19] (also known as Schrieffer–Wolff transformation [2]) to calculate the effective Hamiltonian. If applied directly, this approach requires full diagonalization of the unperturbed Hamiltonian, making it unfeasible in large systems. We find, however, that it is sufficient to only exactly know the states in the interesting subspace, and use hybrid KPM to integrate out the remaining states. This allows us to compute effective models in systems with millions of degrees of freedom, as long as the interesting subspace is small.

2.3.1. LÖWDIN PARTITIONING

We start by separating the initial Hamiltonian into unperturbed part H_0 and perturbation with λ_α as small parameters:

$$H = H_0 + \sum_{\alpha} \lambda_{\alpha} H'_{\alpha}. \quad (2.10)$$

Assuming that the eigenstates and energies of H_0 are known

$$H_0 |\psi_n\rangle = E_n |\psi_n\rangle, \quad (2.11)$$

we split states $|\psi_n\rangle$ into two groups, A and B . We are interested in states from group A whereas the effect of states B we include via perturbation theory. We assume that these two groups of states are separated in energy, but states within A or B may be degenerate. The goal is to find a unitary basis transformation with skew-Hermitian S as

$$\tilde{H} = e^{-S} H e^S, \quad (2.12)$$

such that the transformed Hamiltonian $\tilde{H}$ does not couple the A and B subspaces, and the block in the A subspace is the effective Hamiltonian, $H_{\text{eff}} = \tilde{H}_{AA}$. We find S and H_{eff} order-by-order in the small parameters (for details see Appendix 2.B):

$$H_{\text{eff}} = \tilde{H}^{(0)} + \sum_{\alpha} \lambda_{\alpha} \tilde{H}^{(1,\alpha)} + \sum_{\alpha\beta} \lambda_{\alpha} \lambda_{\beta} \tilde{H}^{(2,\alpha\beta)} + \dots \quad (2.13)$$

When the A subspace corresponds to a single eigenvalue, that is possibly degenerate, the Löwdin perturbation theory reproduces the conventional perturbation theory.

2.3.2. THE KPM APPROXIMATION OF EFFECTIVE HAMILTONIAN

To provide a concrete example, we consider the second-order effective Hamiltonian with one small parameter,

$$H_{\text{eff}} = \tilde{H}^{(0)} + \lambda \tilde{H}^{(1)} + \lambda^2 \tilde{H}^{(2)}, \quad (2.14a)$$

with the explicit terms

$$\tilde{H}_{mn}^{(0)} = E_m \delta_{m,n}, \quad (2.14b)$$

$$\tilde{H}_{mn}^{(1)} = \langle \psi_m | H' | \psi_n \rangle, \quad (2.14c)$$

$$\begin{aligned} \tilde{H}_{mn}^{(2)} = \frac{1}{2} \sum_{l \in B} & \left(\frac{\langle \psi_m | H' | \psi_l \rangle \langle \psi_l | H' | \psi_n \rangle}{E_m - E_l} \right. \\ & \left. + \frac{\langle \psi_m | H' | \psi_l \rangle \langle \psi_l | H' | \psi_n \rangle}{E_n - E_l} \right), \end{aligned} \quad (2.14d)$$

where m and n index states of the A subspace and l indexes states of the B subspace.

We rewrite the first term in the second order contribution as

$$\begin{aligned} & \sum_{l \in B} \frac{\langle \psi_m | H' | \psi_l \rangle \langle \psi_l | H' | \psi_n \rangle}{E_m - E_l} \\ &= \langle \psi_m | H' \left(\sum_{l \in B} \frac{|\psi_l\rangle \langle \psi_l|}{E_m - E_l} \right) H' | \psi_n \rangle \\ &= \langle \psi_m | H' P_B G_0(E_m) P_B H' | \psi_n \rangle, \end{aligned} \quad (2.15)$$

where G_0 is the unperturbed Green's function

$$G_0(E) = \frac{1}{E - H_0} = \sum_i \frac{|\psi_i\rangle\langle\psi_i|}{E - E_i}, \quad (2.16)$$

2

and P_B is the projector onto the B subspace.

This formulation is well suited for approximate evaluation using the KPM expanded Green's function. The Green's function only acts on a small set of vectors, $|\phi_n\rangle = P_B H' |\psi_n\rangle$ for $n \in A$. We obtain the exact eigenstates of the A subspace using sparse diagonalization of H_0 , and compute P_B using $P_B = \mathbb{1} - P_A$. The states $|\phi_n\rangle$ are purely in the B subspace, and we evaluate the Green's function at the energy of a state in the A subspace. The energy separation between the two sets of states removes all divergences so that the action of G_0 is well approximated using KPM with a low energy resolution. After these substitutions, the second-order contribution simplifies to

$$\tilde{H}_{mn}^{(2)} = \frac{1}{2} \langle\phi_m| [G_0(E_m) + G_0(E_n)] |\phi_n\rangle. \quad (2.17)$$

Similar simplification in terms of G_0 is also possible for all higher orders, for details see Appendix 2.C.

2.3.3. EFFECTIVE HAMILTONIAN WITH HYBRID KPM

To accurately approximate the action of G_0 on B states closest to the A subspace in energy, we need to choose the number of Chebyshev moments of the order of W/Δ , where W is the full bandwidth of H_0 and Δ is the gap between A and B states. Hence, for small Δ accurate calculation using KPM becomes computationally expensive. Alternatively, knowing all the B eigenstates would allow exact evaluation of the Green's function, at an even higher computational cost.

To solve this problem, we propose the hybrid KPM approach, where only a subset B_e of the B eigenstates is known explicitly. These we choose to be the eigenstates with closest energy to the A states, and are obtained using sparse diagonalization. We split the Green's function of the B subspace into two terms:

$$G_0(E)P_B = \sum_{l \in B_e} \frac{|\psi_l\rangle\langle\psi_l|}{E - E_l} + G_0^{\text{KPM}}(E)(P_B - P_{B_e}), \quad (2.18)$$

where P_B and P_{B_e} are projectors to the B and B_e subspaces, and G_0^{KPM} is the KPM approximated Green's function.

2.4. COMPUTATION OF THERMODYNAMIC QUANTITIES

2.4.1. EVALUATION OF OPERATOR EXPECTATION VALUES

Physical observables in a non-interacting fermionic system are thermal expectation values of a Hermitian operator $\hat{A}$:

$$\langle\hat{A}\rangle_{E_F} = \sum_k f(E_k, E_F) \langle\psi_k| \hat{A} |\psi_k\rangle, \quad (2.19)$$

where the sum runs over all eigenstates of the Hamiltonian $|\psi_k\rangle$ with eigenenergies E_k . The occupation of the states is given by the Fermi function

$$f(E, E_F) = \frac{1}{e^{\beta(E-E_F)} + 1} \quad (2.20)$$

with $\beta = (k_B T)^{-1}$ and E_F the Fermi energy. Converting the sum to an integral over energy by inserting a delta function, we introduce the spectral density of the operator $A(E) \equiv \text{Tr } \hat{A} \delta(E - \hat{H})$, yielding

$$\langle \hat{A} \rangle_{E_F} = \int dE f(E, E_F) A(E). \quad (2.21)$$

This can be rewritten as a trace using the operator function formalism, and readily evaluated using KPM:

$$\langle \hat{A} \rangle_{E_F} = \text{Tr } \hat{A} f(\hat{H}, E_F) = \sum_m \tilde{\alpha}_m(E_F) \mu_m, \quad (2.22)$$

where the KPM moments are

$$\mu_m = \text{Tr } \hat{A} T_m(\hat{H}). \quad (2.23)$$

The Fermi function changes rapidly in the interval $1/\beta$ around the Fermi level. Our strategy is to compute the states near the Fermi level exactly and approximate the rest of the states using low-order KPM. Following the hybrid KPM approximation, we substitute Eq. (2.9) into Eq. (2.22):

$$\begin{aligned} \langle \hat{A} \rangle_{E_F} &\approx \sum_m \tilde{\alpha}_m(E_F) (\mu_m - \mu_m^A) \\ &+ \sum_{i \in A} f(E_i, E_F) \langle \psi_i | \hat{A} | \psi_i \rangle, \end{aligned} \quad (2.24)$$

where the KPM moments restricted to the A subspace are

$$\mu_m^A = \sum_{i \in A} T_m(E_i) \langle \psi_i | \hat{A} | \psi_i \rangle. \quad (2.25)$$

The trace in the full contribution is efficiently approximated using the stochastic trace approximation [9]. The exact evaluation of the trace is also feasible if the operator $\hat{A}$ has a low rank and the basis of its image space is explicitly known:

$$\mu_m = \sum_{|\psi\rangle \in \text{Im } \hat{A}} \langle \psi | \hat{A} T_m(\hat{H}) | \psi \rangle. \quad (2.26)$$

2.4.2. PERTURBATIVE KPM

We now generalize KPM to allow order-by-order expansion of thermodynamic expectation values. We consider a generic function g and perturbed Hamiltonian $\hat{H} = \hat{H}_0 + \lambda \hat{H}_1$ where λ is a small parameter. Our goal is to evaluate $\text{Tr } g(\hat{H})$ order-by-order in the small parameter. For example, the expectation value of the energy of a filled Fermi sea is $\langle E \rangle = \text{Tr } g(\hat{H})$ with $g(E) = Ef(E, E_F)$. Our method also applies to expressions of the form $\text{Tr } \hat{A} g(\hat{H})$, but we restrict to the $\hat{A} = \mathbb{1}$ case for brevity.

Our idea is to keep track of parameter dependence when computing the Chebyshev recursion relation (2.8), allowing $\hat{H}$ and $|v_m\rangle$ to be polynomials of λ . Since we are only interested in the result up to λ^n order, we discard all higher order terms at every step of the iteration, resulting in KPM moments μ_m and expectation value $\text{Tr } g(\hat{H})$ that is also an n 'th order polynomial of λ . At a finite number of moments M , this method reproduces the series expansion of $\text{Tr } \tilde{g}(\hat{H})$ in λ , where $\tilde{g}$ is the Chebyshev approximation of g . The resulting increase in computational cost scales as $\mathcal{O}(n^2)$, making this method feasible at low expansion orders.

Rearranging the terms in the perturbation expansion allows us to efficiently calculate the trace when the image space of the perturbation H_1 is small. After a cyclic permutation inside the trace, the λ -linear term in the expansion becomes

$$\frac{d}{d\lambda} \text{Tr } g(\hat{H})_{\lambda=0} = \text{Tr } g'(\hat{H}_0) \hat{H}_1, \quad (2.27)$$

where g' is the derivative of g . Because $\hat{H}_1$ is the rightmost operator, the trace reduces to a sum over a basis of the image space of $\hat{H}_1$. Applying this to the energy expectation value in the zero-temperature limit where f is a step function [using that $x\delta(x) = 0$] we get

$$\begin{aligned} \frac{d}{d\lambda} \langle E \rangle_{\lambda=0} &= \frac{d}{d\lambda} \text{Tr } \hat{H} f(\hat{H})_{\lambda=0} \\ &= \text{Tr } f(\hat{H}_0) \hat{H}_1 = \langle \hat{H}_1 \rangle_{\lambda=0} \end{aligned} \quad (2.28)$$

which is the same as the ground state expectation value of H_1 , and was already discussed in the previous section. Similar simplifications apply to all higher orders; here we present the second-order case in detail. For a generic function g and Hamiltonian $\hat{H} = \hat{H}_0 + \lambda \hat{H}_1 + \lambda^2 \hat{H}_2$, by expanding and permuting terms proportional to λ^2 we find

$$\begin{aligned} \frac{1}{2} \frac{d^2}{d\lambda^2} \text{Tr } g(\hat{H})_{\lambda=0} \\ = \text{Tr } g'(\hat{H}_0) \hat{H}_2 + \frac{1}{2} \frac{d}{d\lambda} \text{Tr } g'(\hat{H}) \hat{H}_1_{\lambda=0} \end{aligned} \quad (2.29)$$

To evaluate the traces, we sum over the basis of the image spaces of $\hat{H}_2$ and $\hat{H}_1$ respectively in the two terms. To obtain the second term we use the KPM expansion to first order in λ .

To apply the hybrid KPM approach to the perturbative KPM, we utilize the hybrid KPM Löwdin perturbation theory developed in Sec. 2.3, obtaining the perturbation series of the A subspace eigenenergies. We treat a single eigenpair $(E_k, |\psi_k\rangle)$ of $\hat{H}_0$ as the A subspace for the purposes of Löwdin perturbation theory, and use the rest of the exactly known states as the B_e subspace in the hybrid evaluation of the Green's function. Repeating this for every A eigenstate produces the power series expansions of the perturbed E_k up to the desired order. Combining the perturbative KPM result for the full spectrum and substituting the Löwdin expansion of the A subspace we obtain

$$\text{Tr } g(\hat{H}) \stackrel{\text{hybrid}}{\approx} \text{Tr } \tilde{g}(\hat{H}) - \sum_{k \in A} \tilde{g}(E_k) + \sum_{k \in A} g(E_k). \quad (2.30)$$

We compute the series expansion of the last two terms in λ using the Taylor series of g and $\tilde{g}$. The hybrid Löwdin approximation has the highest accuracy for states in the

middle of the A subspace energy range, which we choose to coincide with the fastest-changing region of g' . For states close to the edge of the A subspace energy range the approximation is less accurate, but, at the same time, the difference between g and $\tilde{g}$ is also small, resulting in a small overall error.

2.5. APPLICATIONS

2.5.1. SUPERCURRENT AND JOSEPHSON INDUCTANCE

As an illustration, we apply the hybrid KPM method to calculate supercurrent in a Josephson junction [10]. When the Thouless energy is smaller than the superconducting gap Δ —the so-called long-junction regime [11, 12]—the continuum spectrum at $|E| > \Delta$ also responds to the superconducting phase difference and contributes to the total supercurrent [20]. In the hybrid KPM approach, we calculate the subgap states using exact diagonalization, and estimate the contribution of continuum states using KPM.

We consider a Josephson junction with a normal region of length L_N , superconducting leads of length L_S and width W as shown in the inset of Fig. 2.1. For simplicity, we consider a spinless Bogoliubov-de Gennes (BdG) Hamiltonian without magnetic field:

$$H_{BdG} = \begin{pmatrix} \frac{\mathbf{p}^2}{2m} - \mu & \Delta(x) \\ \Delta^*(x) & \mu - \frac{\mathbf{p}^2}{2m} \end{pmatrix}, \quad (2.31)$$

with $\mathbf{p}$ the momentum operator, m the effective electron mass, and μ the chemical potential. The superconducting order parameter $\Delta(x)$ is zero in the normal region and Δ in the superconducting leads. We discretize this Hamiltonian on a square lattice with lattice constant a and a nearest neighbour hopping $t = \hbar^2/(2ma^2)$. We introduce the superconducting phase difference ϕ through a Peierls substitution

$$H_{ij} \rightarrow \begin{cases} H_{ij} \exp(i\phi\tau_z/2) & \text{if } i \in L \text{ and } j \in R \\ \exp(-i\phi\tau_z/2) H_{ij} & \text{if } i \in R \text{ and } j \in L, \\ H_{ij} & \text{otherwise} \end{cases} \quad (2.32)$$

with H_{ij} the hopping Hamiltonian between site i and j in the BdG formalism, τ_z the Pauli matrix in particle-hole space. Finally, L and R correspond to the left and right sides of a cut in the normal region parallel to the normal-metal–superconductor interface (see the inset of Fig. 2.1). The current operator across the cut is the derivative of the Hamiltonian with respect to the flux:

$$\hat{I} = \frac{2e}{\hbar} \frac{d\hat{H}}{d\phi}. \quad (2.33)$$

To calculate the KPM contribution to the trace

$$\langle \hat{I} \rangle = \text{Tr} \hat{I} f(\hat{H}), \quad (2.34)$$

we use the basis of the sites next to the cut. All other states are annihilated by the current operator and do not contribute to the current.

Here and in the rest of the manuscript we use the Kwant software package [21] to construct tight-binding Hamiltonians. We consider a Josephson junction of length

$L_N = L_S = 50a$ and width $W = 15a$ and set the parameters $\mu = 0.2t$ and $\Delta = 0.15t$. As explained in sec. 2.4, we calculate the subgap Andreev bound states exactly using sparse diagonalization and treat them as the A subspace. We show the spectral density of the current operator $I(E)$ in Fig. 2.1, where we plot the contributions of subgap and continuum states separately. The KPM spectrum of the current operator vanishes at this resolution with $M = 500$ moments. The contribution of only the continuum states calculated with hybrid KPM is, however, non-vanishing, and the exactly known subgap states contribute Dirac delta peaks.

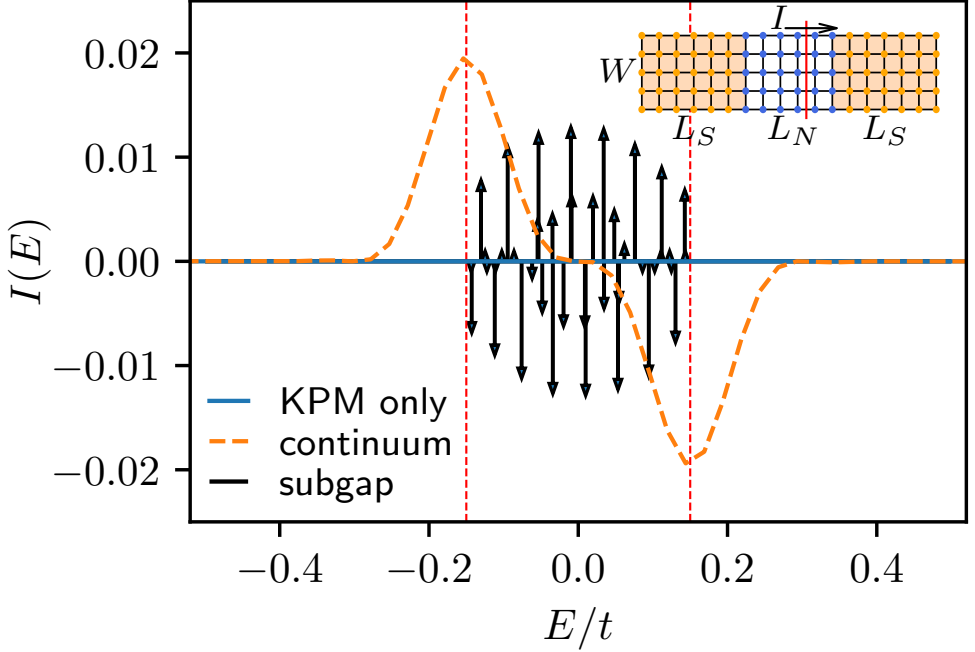


Figure 2.1: Current operator spectrum as a function of energy with the fixed relative superconducting phase of $\pi/2$. The solid blue line represents the KPM-only spectrum of the current operator; the arrows represent the Dirac delta contributions of subgap states; the dashed orange line shows the contribution of the continuum states. Inset: Sketch of the system. The shaded regions are superconducting with a normal region in the middle. The red line represents the cut for which we calculate the supercurrent.

We compute the contributions of the Andreev states and the continuum states to the current-phase relation, with the result shown in Fig. 2.2. The contributions of both the subgap and the continuum states are significant, while their sum agrees with the exact result to high precision.

To demonstrate hybrid KPM in higher-order perturbation theory, we turn to the Josephson inductance. The inverse of the junction inductance is equal to the derivative of the current expectation value with respect to the flux:

$$L_J^{-1} = \frac{(2e)^2}{\hbar^2} \frac{d^2}{d\phi^2} \langle \hat{H} \rangle. \quad (2.35)$$

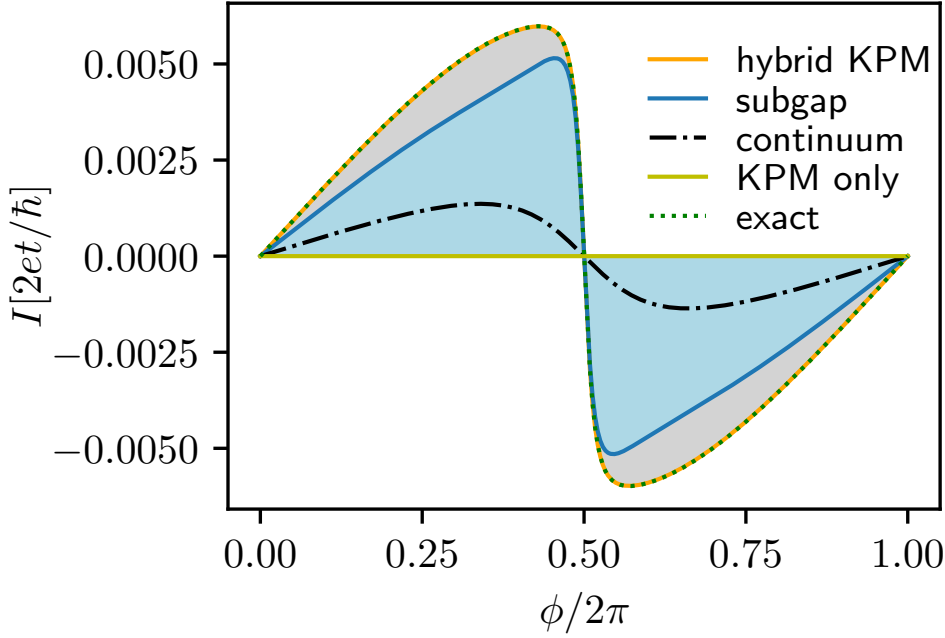


Figure 2.2: Supercurrent as a function of the superconducting phase difference. The orange line is the total supercurrent through a Josephson junction calculated with hybrid KPM, whereas the blue and black lines are the contributions from subgap and continuum states respectively. The hybrid KPM result agrees with full diagonalization, while the pure KPM estimate vanishes.

We evaluate this expression using the hybrid method discussed in Sec. 2.4.2 considering the second derivative of the Hamiltonian, with the result shown in Fig. 2.3. The sharp peak in L_J^{-1} at $\phi = \pi$ is accurately captured by the direct evaluation of the second derivative using our method, while accurate calculation using a discrete derivative of the current expectation value requires a much higher resolution in ϕ . As we observed in Sec. 2.4.2, the hybrid Löwdin perturbation theory estimates the energies of the states near the edge of the A subspace with a low precision. This is why the contribution of the bound states to L_J^{-1} disagrees with the derivative of the bound state contribution to the current shown in Fig. 2.2. Nevertheless, because this error cancels with the B subspace contribution, the precision of the full result remains the same.

The zero-temperature limit is the most computationally expensive both to pure KPM and imaginary energy integration [22, 23]. Computing the finite temperature results within hybrid KPM, however, amounts to replacing f with the Fermi function at the correct temperature. Because the computational cost of hybrid KPM is dominated by the computation of the KPM moments and the perturbation expansion of low-lying states, the extra computational cost of a temperature sweep is negligible.

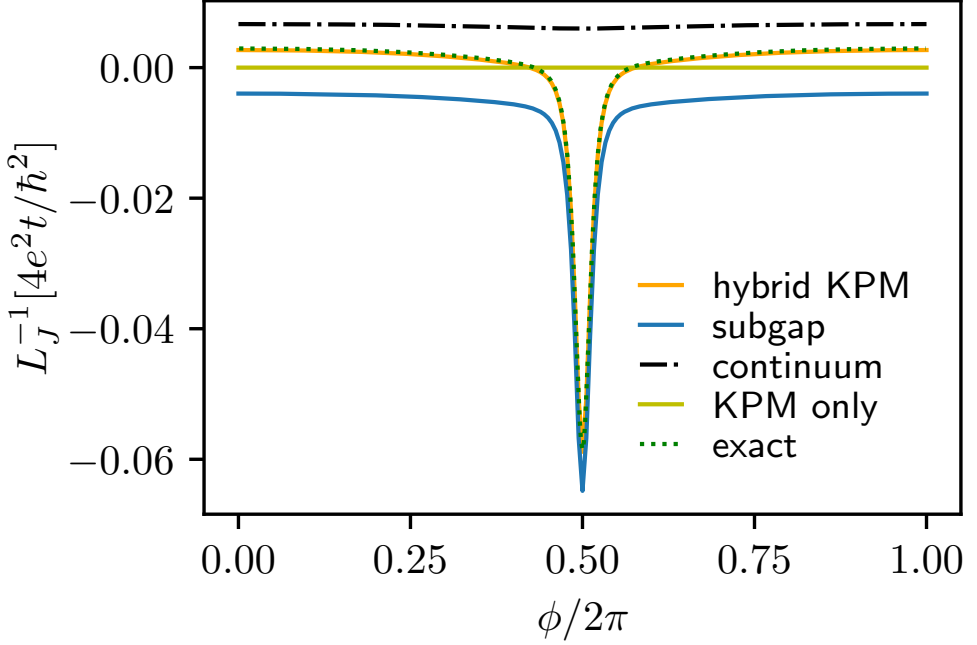


Figure 2.3: Inverse Josephson inductance as a function of the superconducting phase difference. The orange line represents L_J^{-1} calculated with hybrid KPM, whereas the blue and black lines show the corresponding contributions from subgap and continuum states respectively. The hybrid KPM result agrees with the exact result using full diagonalization, while the pure KPM result vanishes.

2.5.2. EFFECTIVE DOUBLE QUANTUM DOT HAMILTONIAN

Turning to the hybrid Löwdin perturbation theory, we apply hybrid KPM to calculate an effective Hamiltonian of several low energy states in a double quantum dot system. To use the basis of individual quantum dot states, we start with a system with decoupled dots and include hoppings between the dots perturbatively. When the tunnel barrier between the dots is low, the eigenstates become strongly hybridized, so that the perturbation theory requires a sufficiently high order in the inter-dot coupling. We address this need by including the eigenfunctions and eigenenergies of the lowest few bound states exactly and treating the remaining part of the energy spectrum up to the third-order in the Löwdin perturbation theory using the hybrid KPM approach.

We consider two gate-defined quantum dots formed in a quantum well with the interdot tunnel coupling and dot chemical potential controlled by the gate electrodes. In the continuum approximation the quantum well Hamiltonian is

$$H_{2D} = \frac{\hbar^2}{2m_e} (k_x^2 + k_y^2) + V(x, y), \quad (2.36)$$

where m_e is the effective electron mass, k_x and k_y are the components of the electron wave vector, and $V(x, y)$ is the electrostatic potential. We discretize the continuum Hamiltonian H_{2D} using the finite difference approximation on a square lattice with a lattice constant of

5 nm and the effective mass of GaAs. We consider the gate geometry of Ref. [13], with the gate electrodes 60 nm above the quantum well. Plunger gates control the dot chemical potential, while the tunnel barrier height between the dots is controlled by the barrier gate in the middle, as shown in Fig. 2.4. We calculate the electrostatic potential induced in the quantum well using the approximation of Ref. [24]. In the initial configuration, the gate potentials form two tunnel-coupled quantum dots, as shown in Fig. 2.4.

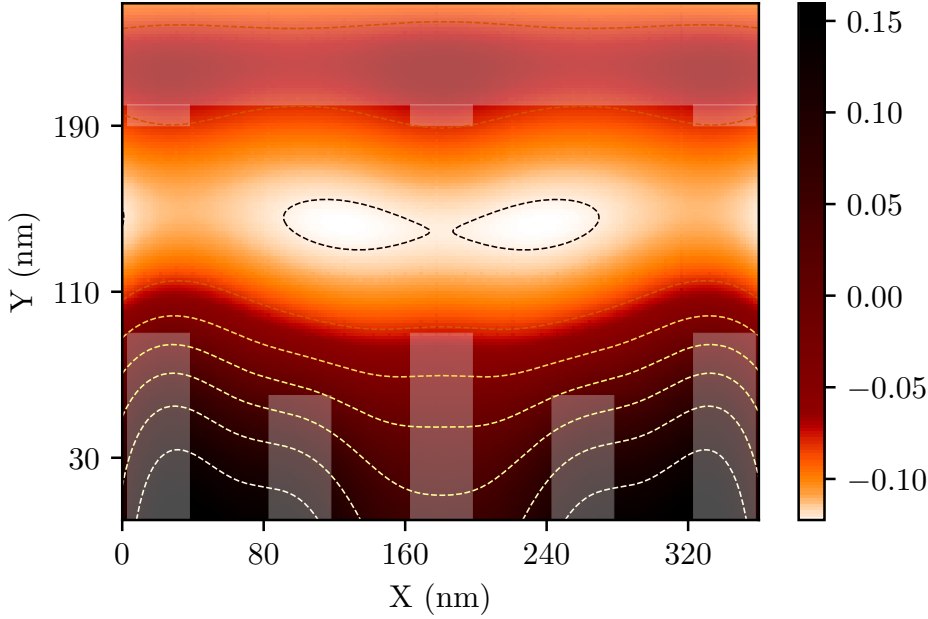


Figure 2.4: The 2DEG electrostatic potential superimposed with gate electrodes deposited on top of the GaAs heterostructure. We use the gate design and heterostructure from [13]. Plunger and barrier gates are shown at the bottom and screening gates at the top. By applying a negative voltage to the gate electrodes, we locally deplete the 2DEG to form two quantum dots as represented by the equipotential lines.

We separate the Hamiltonian into a sum of unperturbed H_0 term and two perturbation terms:

$$H = H_0 + \lambda_g \Delta H_g + \lambda_c H_c. \quad (2.37)$$

Here H_0 is the initial Hamiltonian with the hoppings between the left and the right halves of the system removed, ΔH_g is the deviation of the gate potential from the initial setting, and H_c is the hoppings connecting the left and right halves. We split the spectrum of the Hamiltonian into two subspaces: A contains the two lowest bound states in each quantum dot, and B the rest of the energy spectrum. We obtain the states in A and a few states in $B_e \subset B$ with the lowest energies using sparse diagonalization. Setting $\lambda_c = 1$ reproduces the original Hamiltonian without the cut between the dots. We select the perturbation ΔH_g as the potential resulting from an antisymmetric detuning of the plunger gates by $\pm \Delta V/2$. In Fig. 2.5, we compare the eigenenergies calculated from the effective model using first and third-order perturbation theory with the sparse diagonalization results.

The first-order perturbation does not require hybrid KPM and coincides with conventional first-order perturbation theory. It cannot, however, accurately estimate the spectrum, while third-order Löwdin perturbation theory using hybrid KPM shows a good agreement with the exact result.

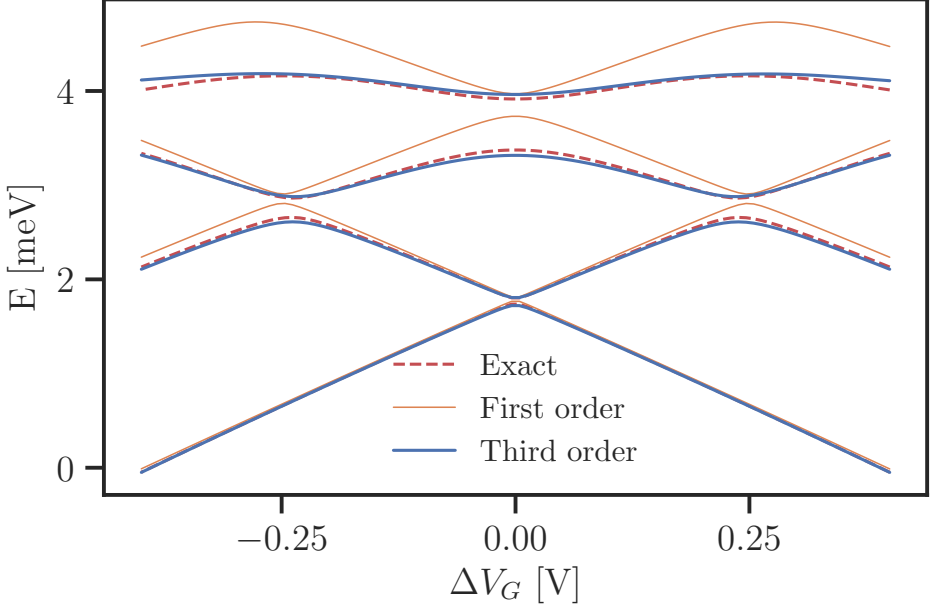


Figure 2.5: Energy spectrum as a function of the gate voltage difference between the two dots. Eigenenergies calculated from the first and third-order effective models are compared against the exact energies.

2.5.3. EFFECTIVE BAND STRUCTURES

Semiconductor nanowires, besides many potential applications [14], are of interest as a platform to realize Majorana states when proximitized with a superconductor [15–17]. The necessary ingredients for the creation of Majorana states are spin-orbit interaction and external magnetic field, which remove spin degeneracy in the lowest subband of the wire, resulting in effective p -wave superconducting pairing. In an external electric field normal to the wire the bulk spin-orbit coupling of the semiconductor results in Rashba spin-orbit interaction. The minimal model describing the relevant phenomena, except for superconductivity, is the 2-band effective model:

$$H = \frac{\hbar^2}{2m^*} k_z^2 + \mu + \alpha k_z (\sigma_y E_x + \sigma_x E_y) + \mu_B \mathbf{B} g \boldsymbol{\sigma}, \quad (2.38)$$

where m^* is the effective mass of the lowest subband, k_z is the momentum along the wire, μ is the chemical potential, E_x and E_y are components of the electric field, $\boldsymbol{\sigma}$ are the Pauli matrices and α is the strength of the Rashba spin-orbit interaction. The external

magnetic field is $\mathbf{B}$, μ_B is the Bohr-magneton and g is the effective g -factor tensor in the lowest subband. While this simple model is easy to solve, extracting the parameters of realistic setups starting from a microscopic model is computationally hard. We solve this task using hybrid KPM.

We start from the 8-band $\mathbf{k} \cdot \mathbf{p}$ model of bulk zinc-blende materials, in particular InAs [4, 19, 25, 26]. This continuum model accurately captures the s -type conduction and p -type valence bands near the Fermi level at small momenta, up to second-order in k . We consider an infinite wire oriented along the z -axis with an approximately circular cross-section in the xy plane with radius R . We discretize the $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian in the xy -plane by replacing momenta k_x and k_y (but not k_z) with discrete spatial derivatives. We include the Zeeman term with the bulk g -factor $g^* = -15$ of InAs [4, 27]. We introduce the orbital magnetic field using Peierls substitution, as well as the electrostatic potential $V = -E_x x - E_y y$. For this example, we use radius $R = 25$ nm with discretization grid lattice constant $a = 1$ nm. This results in a tight-binding model with 31056 degrees of freedom, outside of the practical limits of full diagonalization on a single computer.

We use the Löwdin algorithm treating the tight binding Hamiltonian with vanishing external fields and $k_z = 0$ as the unperturbed Hamiltonian, and include perturbations up to second order in k_z and the electric field, and up to linear order in the magnetic field. Using second-order perturbation theory, we obtain the effective model of the form (2.38) with $m^* = 0.023m_0$, $\alpha = 2.67 \text{ nm}^2$, $\mu = 0.43 \text{ eV}$, $g_{xx} = g_{yy} = -15.4$ and $g_{zz} = -15.5$, with m_0 the free electron mass and all other terms approximately vanishing. This perturbative treatment, only accurate at small parameter values, does not capture the overall energy shift of the subbands resulting from the electrostatic field at field strengths relevant to experiments. Hence, we also construct the effective model using $E_{x0} = 10 \text{ meV/nm}$ as the unperturbed Hamiltonian. The resulting spectrum at finite k_z and B_z agrees with the exact eigenenergies of the full model as illustrated in Fig. 2.6.

2.6. CONCLUSIONS

We developed the hybrid kernel polynomial method, where we combine the strengths of KPM in treating many states at a low energy resolution and of sparse diagonalization in treating a few states with high accuracy. We applied this method to the problems of accurate calculation of expectation values, perturbation theory of thermodynamic quantities, and construction of perturbative effective models. The source code of these general and reusable algorithms is available at [28], together with the source code and data of the examples showcased in the manuscript.

We applied our method to several active research topics in condensed matter and mesoscopic physics: the calculation of supercurrent and inductance in a Josephson junction, the design of spin qubits defined in a two-dimensional electron gas, and the calculation of the effective band structure in a realistic model of a semiconductor nanowire. Our examples illustrate how the combination of low and high resolutions enables the investigation of response functions and effective models in systems whose size would make this prohibitively expensive using other approaches.

We have not yet addressed the following relevant questions:

- What is the optimal way to choose the number of the exactly calculated states

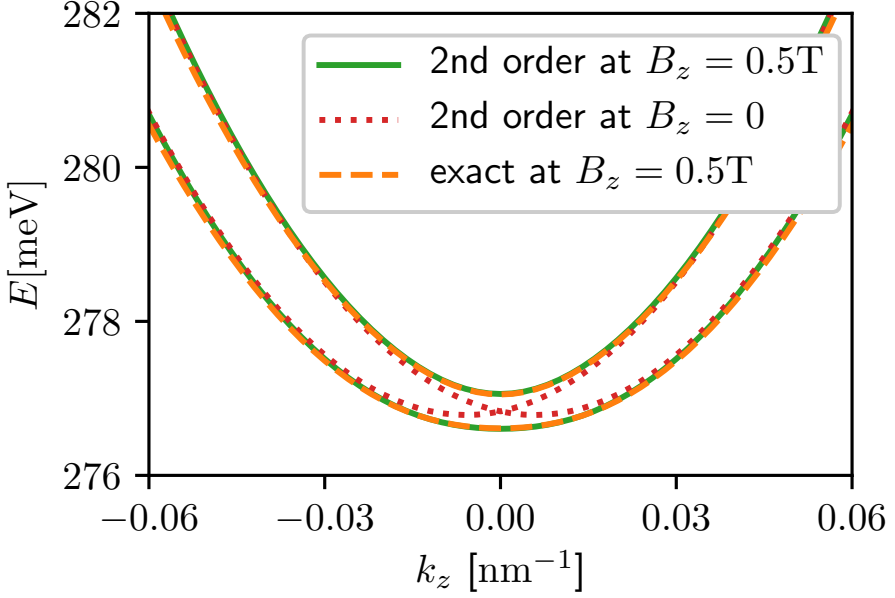


Figure 2.6: Energy spectrum of the lowest subband of an InAs nanowire of radius 5 nm. The plot shows the exact result from sparse diagonalization with $B_z = 0.5\text{T}$ and $E_x = 10\text{ meV/nm}$, and the perturbation theory result around $E_{x0} = 10\text{ meV/nm}$ at 2nd order at $B_z = 0$ and $B_z = 0.5\text{T}$.

and the number of moments in hybrid KPM to minimize the computational effort required for given precision?

- How quickly does the stochastic trace approximation converge in the perturbative KPM scheme?
- What is the general form of rearranged equations similar to (2.29) for higher orders and multiple perturbation parameters?
- How does the efficiency of our method compare to other recursive numerical approaches to perturbation theory, such as Ref. [29]?

These we leave to future work.

Because our method allows the treatment of Hilbert spaces up to millions of degrees of freedom, we expect it to be useful in treating interacting quantum mechanical problems. We conjecture that the hybrid approach will also improve KPM-assisted self-consistent mean-field [30] and density matrix renormalization group [31, 32] calculations. Accurate simulation of nanoelectronic devices with truncated few-electron Hilbert spaces is also a promising future direction of research using this methodology.

ACKNOWLEDGEMENTS

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AUTHOR CONTRIBUTIONS

A. R. Akhmerov and P. M. Perez-Piskunow proposed the idea of hybrid KPM and initiated the project. P. M. Perez-Piskunow implemented the conventional KPM algorithms. M. Wimmer proposed and R. Skolasinski implemented the automated Löwdin perturbation theory using full diagonalization. M. Wimmer proposed using KPM for Löwdin perturbation theory, P. M. Perez-Piskunow and D. Varjas implemented hybrid Löwdin perturbation theory. S. R. Kuppaswamy applied Löwdin perturbation theory to the spin qubit example. D. Varjas and R. Skolasinski applied Löwdin perturbation theory to the nanowire example. P. M. Perez-Piskunow and M. Irfan implemented the hybrid expectation value calculation. D. Varjas proposed and implemented the hybrid expectation value perturbation theory. M. Irfan applied these methods to the Josephson junction example. A. R. Akhmerov and M. Wimmer oversaw the project and the code development. All authors took part in writing the manuscript.

2.A. CHEBYSHEV POLYNOMIAL EXPANSION OF SELECTED FUNCTIONS

We explicitly give the expansion of a few common functions used in condensed-matter physics and this manuscript: Dirac delta function (used in spectral densities):

$$\delta(E - \hat{H}) = \frac{1}{\pi\sqrt{1-E^2}} \sum_m \frac{2}{1+\delta_{m,0}} T_m(E) T_m(\hat{H}). \quad (2.39)$$

The Green's functions:

$$G^\pm(E, \hat{H}) = \lim_{\eta \rightarrow 0^+} \frac{1}{E - \hat{H} \pm \eta i} = \mp \frac{2i}{\sqrt{1-E^2}} \sum_m \frac{1}{1+\delta_{m,0}} \exp(\pm i m \arccos(E)) T_m(\hat{H}). \quad (2.40)$$

2.B. DETAILS OF LÖWDIN EXPANSION

We adapt this section from Refs. [19] and [34], that closely follows the derivation of arbitrary order quasi-degenerate perturbation theory in Ref. [4]. The goal is to find a unitary basis transformation (Schrieffer–Wolff transformation) with skew-Hermitian matrix S ($S^\dagger = -S$) as

$$\tilde{H} = e^{-S} H e^S, \quad (2.41)$$

such that the transformed Hamiltonian $\tilde{H}$ does not couple the A and B subspaces. The transformation should be the identity when the perturbation vanishes and we expand S

as a series in successive orders of the perturbation

$$S = \sum_{j=1}^{\infty} \lambda^j S^{(j)}. \quad (2.42)$$

2

The transformed Hamiltonian (using the Baker-Campbell-Hausdorff formula) is

$$\tilde{H} = \sum_{j=0}^{\infty} \frac{1}{j!} [H, S]^{(j)} = \sum_{j=0}^{\infty} \frac{1}{j!} [H_0 + \lambda H'_d, S]^{(j)} + \sum_{j=0}^{\infty} \frac{1}{j!} [\lambda H'_n, S]^{(j)}, \quad (2.43)$$

where the nested commutator $[A, B]^{(j)}$ is defined as

$$[A, B]^{(j)} = [\dots [A, \underbrace{B, \dots, B}_{j \text{ times}}], \quad (2.44)$$

with commutator $[A, B] = AB - BA$ and we split the perturbation into block-diagonal and block off-diagonal parts as $H' = H'_d + H'_n$ with with $(H'_d)_{AB} = (H'_d)_{BA} = (H'_n)_{AA} = (H'_n)_{BB} = 0$ (X_{AB} denotes the restriction of operator X to the AB block). The requirement on the S we seek is $\tilde{H}_{AB} = \tilde{H}_{BA} = 0$ and we call $\tilde{H}_{AA}$ the effective Hamiltonian. We choose S to be block off-diagonal such that $S_{AA} = S_{BB} = 0$, this removes arbitrary unitary transformations within the A and B subspaces from the result.

To do n 'th order perturbation theory we demand the equations to be satisfied for all terms up to λ^n . Separating terms that contribute to diagonal and off-diagonal terms ($\tilde{H} = \tilde{H}_d + \tilde{H}_n$ with $(\tilde{H}_d)_{AB} = (\tilde{H}_d)_{BA} = (\tilde{H}_n)_{AA} = (\tilde{H}_n)_{BB} = 0$) we find:

$$\tilde{H}_d = \sum_{j=0}^{\infty} \frac{1}{(2j)!} [H_0 + \lambda H'_d, S]^{(2j)} + \sum_{j=0}^{\infty} \frac{1}{(2j+1)!} [\lambda H'_n, S]^{(2j+1)}, \quad (2.45a)$$

$$\tilde{H}_n = \sum_{j=0}^{\infty} \frac{1}{(2j+1)!} [H_0 + \lambda H'_d, S]^{(2j+1)} + \sum_{j=0}^{\infty} \frac{1}{(2j)!} [\lambda H'_n, S]^{(2j)}. \quad (2.45b)$$

Our goal is to recursively find $S^{(n)}$ from the lower orders $S^{(j)}$ for $j \in [1 \dots n-1]$. We solve $\tilde{H}_n = 0$ up to n 'th order by inserting the expansion $S = \sum_{j=1}^n \lambda^j S^{(j)}$ into (2.45b) and letting the sums in j run to $\lfloor (n-1)/2 \rfloor$, this produces all terms up to n 'th order. We observe that at n 'th order $S^{(n)}$ only appears in a single commutator, allowing to rearrange the n 'th order terms in the equation $\tilde{H}_n = 0$ as

$$[H_0, S^{(n)}] = Y^{(n)} \quad (2.46)$$

where $Y^{(n)}$ only depends on lower orders of S . We generate the Y 's using symbolic computer algebra. The first few terms are:

$$[H_0, S^{(1)}] = Y^{(1)} = -H'_n, \quad (2.47a)$$

$$[H_0, S^{(2)}] = Y^{(2)} = -[H'_d, S^{(1)}], \quad (2.47b)$$

$$[H_0, S^{(3)}] = Y^{(3)} = -[H'_d, S^{(2)}] - \frac{1}{3} [[H'_n, S^{(1)}], S^{(1)}]. \quad (2.47c)$$

As the Y 's are purely off-diagonal Hermitian, it is possible to write only $Y_{AB}^{(n)}$ in terms of S_{AB} , S_{BA} and the restricted components of H .

The equations (2.47) can be iteratively solved as

$$S_{ml}^{(j)} = \frac{Y_{ml}^{(j)}}{E_m - E_l} \quad (2.48)$$

where indices m and l correspond to states in the A and B subspace respectively. With the $n-1$ order expansion of S at hand, we substitute it into (2.45a) with the sum over j running to $\lfloor n/2 \rfloor$, or directly into (2.43) with the sum over j running to n , to produce $\tilde{H}_d$ up to n 'th order.

The same algorithm works in the case of multiple expansion parameters by replacing $\lambda H'$ with $\sum_\alpha \lambda_\alpha H'_\alpha$ and only keeping track of terms with total power j in the λ_α in $S^{(j)}$ and $Y^{(j)}$. Finally, we write the AA block of the transformed Hamiltonian as a sum of successive orders of the perturbation to obtain the effective Hamiltonian:

$$H_{\text{eff}} = \tilde{H}^{(0)} + \sum_\alpha \lambda_\alpha \tilde{H}^{(1,\alpha)} + \sum_{\alpha\beta} \lambda_\alpha \lambda_\beta \tilde{H}^{(2,\alpha\beta)} + \dots \quad (2.49)$$

2.C. USING KPM IN HIGHER ORDER LÖWDIN EXPANSION

To use KPM efficiently, we want to avoid using an explicit basis for the B subspace. We observe that the expressions (2.47) for Y and (2.45a) for $\tilde{H}_{AA}$ can be expanded in terms of the restricted operators (i.e. H'_{AA} , H'_{AB} , etc.). Whenever two terms with A indices are adjacent, we may insert a projector onto the A states $P_A = \sum_m |m\rangle\langle m|$ with a full basis of A states $|m\rangle$. Whenever two terms with B indices are adjacent, we insert a projector onto the B subspace $P_B = \mathbb{1} - \sum_m |m\rangle\langle m|$. This allows to remove the restriction from one of the adjacent terms, for example

$$\langle m | S_{AB} H'_{BB} S_{BA} | m' \rangle = \langle m | P_A S P_B P_B H' P_B P_B S P_A | m' \rangle = \langle m | S H' S | m' \rangle = \sum_{ij} S_{mi} H'_{ij} S_{jm'} \quad (2.50)$$

where we used that S is only nonzero in the off-diagonal blocks. This allows to only store the mixed matrix elements $S_{mi} = \langle m | S | i \rangle$ where $|i\rangle$ is the original basis where the Hamiltonian is sparse with indices i, j running over the full Hilbert space, and $|m\rangle$ is the basis of the A subspace. In this basis $\sum_i S_{mi} (P_B)_{ij} = S_{mj}$, similarly for block off-diagonal matrices. It is possible to replace all H_{BB} terms with H because there is only one H in every product, all the other terms are S 's. This is advantageous as H' acting on the full Hilbert space of size N can be represented as a sparse matrix of $\mathcal{O}(N)$ nonzero entries, while S_{mi} and other off-diagonal components can be stored as small dense matrices with $\mathcal{O}(Na)$ entries where $a = \dim(A)$.

Now we rewrite (2.48) in terms of the Green's function:

$$S_{mi}^{(n)} = \sum_j Y_{mj}^{(n)} \left(\frac{1}{E_m - H_0} \right)_{ji} = \sum_j \left[G_0(E_m)_{ij} \left(Y^{(n)\dagger} \right)_{jm} \right]^\dagger \quad (2.51)$$

where we used that Y is block off-diagonal and $G_0(E)$ does not mix the A and B subspaces. For numerical stability reasons, we still apply P_B from the right in practice. Following the

procedure outlined in Appendix 2.B we successively generate all S terms and produce $\tilde{H}_{AA}$, the only difference is using the above basis convention.

The computational complexity of generating the n 'th order effective Hamiltonian (in the case of a single small parameter) is $\mathcal{O}(n^2 aNM)$, where M is the number of KPM moments, practically chosen to be at the order of bandwidth/gap. We obtain this estimate by the following reasoning: A single evaluation of the KPM Green's function on a vector costs $\mathcal{O}(NM)$. To get $S^{(j)}$, we need to apply G to (aj) vectors on the right hand side, as $Y^{(j)}$ is a j 'th order polynomial of the small parameter. We argue that the KPM step is the costliest part of the procedure, because evaluation of Y and $\tilde{H}$ only involves products of small or sparse matrices.

There is, however, a combinatorial factor in the number of terms involved in these expressions, which grows exponentially with j . At high orders $Y^{(n)}$ contains $\mathcal{O}(2^n)$ terms with a single small parameter. At high enough orders, it is more efficient to directly evaluate the commutator series giving $Y^{(n)}$ by substituting the $n-1$ order expansion of S with numerical coefficients. Truncating to terms of at most order n after every multiplication, this only takes $\mathcal{O}(n^3)$ time. Hence, this latter method becomes more efficient for high enough orders. Combinatorial factors are even larger if there are multiple small parameters in the expansion. We defer further analysis of the complexity and possible optimizations of high order expansions.

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3

IMPACT OF DISORDER ON THE DISTRIBUTION OF GATE COUPLING STRENGTHS IN A SPIN QUBIT DEVICE

This chapter has been previously published as Sathish R. Kuppuswamy, Hugo Kerstens, Chun-Xiao Liu, Lin Wang, and Anton Akhmerov, *Impact of disorder on the distribution of gate coupling strengths in a spin qubit device*, arXiv:2208.02190. I defined the project goal, set-up numerical simulations, collected experimental data, compared numerical results to experimental data, supervised Hugo Kerstens to simulate non-planar gate design and wrote manuscript.

3.1. INTRODUCTION

Spin qubits are an actively developed platform for building a quantum computer with both single- and two-qubit gate fidelity exceeding the error threshold required for achieving fault tolerance [1–3]. In general, this approach follows the Loss and DiVincenzo proposal [4] and traps single electrons in an array of coupled quantum dots. Time-dependent manipulation of chemical potentials and quantum dot couplings using plunger and barrier electrostatic gates implements coherent operations on the electron spins—the quantum gates [5]. Prototype implementations of a few quantum dot devices were demonstrated in several material platforms, for example in GaAs [5–8], Si/SiGe [9–12], Ge/SiGe [13, 14] and Si/SiO₂ [15–17] heterostructures.

To go beyond a few qubit devices, ongoing effort is invested into designing and operating larger-scale quantum dot arrays [8, 12, 18] necessary to implement more complex quantum circuits without compromising qubit performance. For example, the change from GaAs to Si avoids decoherence due to the hyperfine coupling to the nuclear spins [19]. Because the electron effective mass is larger in Si, the electrostatic gates must be smaller and closer to each other due to the higher electron localization [11, 12]. Another ongoing development—2D quantum dot arrays [8, 14]—improves qubit connectivity, and more directly corresponds to the error-correcting codes. Although such new designs are vital for future progress, they require going beyond the state of the art in device complexity and precision.

Spin qubit gate designs are commonly characterized by performing the full experimental cycle: fabricating, tuning, and then measuring the device. This pipeline can be partially tested using numerical simulations [20]. Numerical simulations begin with discretizing the continuum Hamiltonian which describes the two-dimensional (2DEG) electron gas in a semiconductor heterostructure. The potential landscape of the 2DEG is shaped to host quantum dots by optimizing the electrostatic environment using non-linear optimizers. In this process, electrostatic potential due to gates is calculated by solving Poisson's equation. Finally, the discretized Hamiltonian is diagonalized to obtain eigenenergies and eigenvectors of the electron states confined in quantum dots. Numerical simulations, despite being complex and demanding, require no longer than days to run, and therefore they are still much faster than fabrication and measurement that lasts months.

Structural variation due to the fabrication as well as electrostatic disorder [21, 22] limits the usefulness of numerical simulations. In addition, although gates are designed to predominantly control only one parameter, changing the voltage of one plunger or barrier gate affects all the dot Hamiltonian parameters instead of a single chemical potential or a tunnel coupling [23]. Because of these complications, a significant amount of effort is dedicated to automating the tuning of an experimental device using either an effective model combined with a measurement protocol [23] or using a more general machine learning techniques [24–27].

The final tuning step determines the *virtual gates* [23]—linear combinations of physical gates that couple to a single quantum dot Hamiltonian parameter—that enable efficient time-dependent manipulation of spin qubit devices [28]. Here we demonstrate that such gate coupling strengths are efficiently predicted by numerical simulations even in the presence of disorder. We also provide a reference implementation for perform-

ing this procedure, available at [29]. Our simulation of an experimental device agrees with the measurements up to the expected uncertainty due to electrostatic disorder. We also demonstrate the flexibility of our approach by applying it to a non-planar geometry inspired by a FinFET transistor setup [17, 30]. Furthermore, by implementing relevant optimizations, we can reduce the simulation time of a single device to a few minutes of CPU time.

3.2. METHODS

In the continuum approximation, the Hamiltonian of the 2DEG confined in a semiconductor heterostructure is

$$H_{2D} = -\frac{\hbar^2}{2m_e} \left(\partial_x^2 + \partial_y^2 \right) + U(x, y), \quad (3.1)$$

where m_e is the effective mass and $U(x, y)$ is the gate-defined electrostatic potential. We ignore the spin degree of freedom in this work and only focus on finding the relation between gate potential and electrostatic potential of the 2DEG in the presence of disorder. We further discretize Eq. (3.1) on a two-dimensional regular grid with nearest-neighbor hoppings to form the tight-binding Hamiltonian H .

Electrostatic potential $U(\mathbf{r})$ is a solution to the Poisson's equation

$$\nabla \cdot [\epsilon_r(\mathbf{r}) \nabla U(\mathbf{r})] = -\frac{\rho(\mathbf{r})}{\epsilon_0}, \quad (3.2)$$

where ϵ_0 is the vacuum permittivity, and ϵ_r is the relative permittivity. We apply Dirichlet boundary conditions with potential V_i at the i -th gate electrode boundary and $V = 0$ at the simulation boundary. The source term $\rho(\mathbf{r})$ is the charge density which only includes the possible impurity charges

$$\rho(\mathbf{r}) = \sum_{\mathbf{r}_c} e \delta(\mathbf{r} - \mathbf{r}_c), \quad (3.3)$$

where the summation is carried out over all the positions $\mathbf{r}_c$ of the charged impurities, and e is the elementary charge. Because we are interested in the single particle Hamiltonian, we neglect the interaction of electrons in different quantum dots, which can be added at later steps. This makes the Poisson equation linear. To reduce the finite-size effects, we simulate a sufficiently large volume surrounding the sample. We use the electrostatic solver of Ref. [31] to construct the finite volume mesh of the simulation area and solve the discretized Poisson equation. To improve performance, we use a coarser grid in the empty space. The general solution of Eq. (4.1) is

$$U(\mathbf{r}) = U_0(\mathbf{r}) + \sum_k V_k U_k(\mathbf{r}), \quad (3.4)$$

where $U_0(r)$ is the solution with all $V_k = 0$, and $U_0(r) + U_k(r)$ is the solution with $V_l = \delta_{kl}$ and δ the Kronecker symbol. Recasting the solution in this form allows us to compute the LU-decomposition of the Laplace operator once, and apply it only once per gate electrode and impurity charge distribution.

We transform the lowest few eigenstates of H that correspond to the ground state of each dot into a maximally localized form along x with the projected position operator

$$\hat{\mathbf{P}}_x = \langle \psi_i | \hat{\mathbf{X}} | \psi_j \rangle, \quad (3.5)$$

where $1 \leq i, j \leq N$, with N the number of quantum dots. The matrix W diagonalizing $\hat{\mathbf{P}}_x$ is the transformation to the basis of the Wannier orbitals maximally localized in the x -direction, with the eigenvalues x_i of $\hat{\mathbf{P}}_x$ being the Wannier centers—the expected x -positions of these orbitals. We compute the effective Hamiltonian for the quantum dots in the basis of Wannier functions using

$$H_{\text{dots}} = W^\dagger D W, \quad (3.6)$$

where D is a diagonal matrix with N lowest eigenvalues of H . Reformulating the Hamiltonian H into the sum of a constant term H_0 and the term H_{V_k} which changes as a function of the gate k

$$H = H_0 + \sum_k H_{V_k} \Delta V_k, \quad (3.7)$$

allows us to compute the onsite and off-diagonal elements of H_{dots} as a function of the gate voltages

$$\begin{aligned} H_{\text{dots}} = & \sum_i \left(\mu_i + \sum_k \frac{\delta \mu_i}{\delta V_k} \Delta V_k \right) |i\rangle \langle i| \\ & + \sum_{i,j} \left(t_{ij} + \sum_k \frac{\delta t_{ij}}{\delta V_k} \Delta V_k \right) |i\rangle \langle j|, \end{aligned} \quad (3.8)$$

where μ_i is the chemical potential of dot i and t_{ij} is the tunnel coupling between the nearest-neighboring dots i and j . The partial derivatives $\delta \mu_i / \delta V_k$ and $\delta t_{ij} / \delta V_k$ are the coupling strengths between the k -th gate and the i -th chemical potential and the $i j$ -th interdot tunnel coupling respectively.

To tune the device into the optimal operating region, we numerically optimize the gate voltages $\mathbf{V}$ to trap a single electron state in each quantum dot and to set all interdot couplings to the same value. We achieve this result using the cost function

$$f(\mathbf{V}) = \sum_i \left[\frac{1}{t_0} (\mu_i(\mathbf{V}) - \mu_0) \right]^2 + \log^2 \left[\frac{t_{i,i+1}(\mathbf{V})}{t_0} \right], \quad (3.9)$$

where μ_0 is the desired chemical potential and t_0 is the desired interdot tunnel coupling. Since t varies exponentially as a function of the barrier height [28], we apply the natural logarithm to the tunnel couplings in Eq. (3.9), to make the relative significance of two contributions to the cost function comparable.

In the presence of charge impurities in concentrations expected in realistic devices, the optimization using the cost function of Eq. (3.9) fails to tune the device into the proper tunneling regime or even form quantum dots due to the highly nonlinear nature of the problem. To enable convergence in the presence of disorder we add the disorder potential

H_{dis} with a Lagrange multiplier $H_{\text{dis}}\alpha$ to Eq. (3.7) and add $(\alpha - 1)^2$ to the cost function. In addition, we optimize dots to be confined to specific regions by using soft thresholds

$$S(x, \delta x) = \begin{cases} (|x| - \delta x)^2 & \text{for } |x| > \delta x, \\ 0 & \text{otherwise,} \end{cases} \quad (3.10)$$

where δx is the desired range. Combining all terms, we end up with the regularized cost function

$$f'(V) = f(V) + (\alpha - 1)^2 + \sum_i [S(x_i(V) - x_{i0}, \delta x) + S(y_i(V) - y_0, \delta y)], \quad (3.11)$$

with y_i the y -coordinate of i -th Wannier orbital, (x_{i0}, y_0) is the desired position of i -th dot center, and $(\delta x, \delta y)$ the dot position tolerance. Optimizing $f'(V)$ has a high success rate and converges close to the tuned point in the majority of cases. We follow the optimization of f' with an additional optimization of f to ensure that the final configuration corresponds to $\alpha = 1$.

3.3. RESULTS

3.3.1. PLANAR GEOMETRY

We benchmark the numerical simulations by comparing them with the measured data of silicon-doped GaAs/AlGaAs heterostructure measured in Ref. [28]. This device consists of a 2DEG with a dopant density of $1.9 \times 10^{11} \text{ cm}^{-2}$. We approximate the electron density of the undepleted 2DEG—the region away from the dots and the gates—to be equal to the dopant density. Plunger and barrier gates are deposited at 90 nm above the 2DEG to selectively deplete the 2DEG and form quantum dots. Plunger gates mainly couple to μ_i , while barrier gates control t_{ij} . Following Ref. [28] we consider four plunger gates (P1 to P4) and five barrier gates (B1 to B5) to form an array of four quantum dots. We numerically optimize the gate voltages to trap a single electron in each quantum dot and tune t_{ij} to the experimental operating point. The 2DEG electrostatic potential of a tuned clean device is shown in Fig. 3.1.

Following the analysis of Ref. [32], we focus on the dopant charge distribution as the main source of disorder. We simulate the dopants by making the charge of the mesh volumes in the dopant layer Poisson-distributed random variables with the average charge density equal to the dopant density and consider 200 disorder realizations. The target Hamiltonian for the optimization has $\mu_i = 0 \text{ eV}$ (assuming the Fermi energy in the 2DEG is at 0 eV) and all the interdot couplings are set to $20 \mu\text{eV}$. The optimization converges to the desired result in 65% of disorder realizations. While it is likely that further improvements to the optimization algorithm would increase the convergence rate, we consider this performance sufficient since we expect that this value is higher than the experimental yield—the percentage of devices that could be tuned to the proper operating regime compared to the total number of devices attempted in the experiments. The positions of the dot centers in the converged samples exhibit a variation comparable to the dot size, as shown in Fig. 3.2. We benchmark our numerical simulations by comparing the gate voltages and the gate coupling strengths with the experimentally measured ones in Fig. 3.3 and Fig. 3.4 respectively. While the operating point varies strongly across disorder

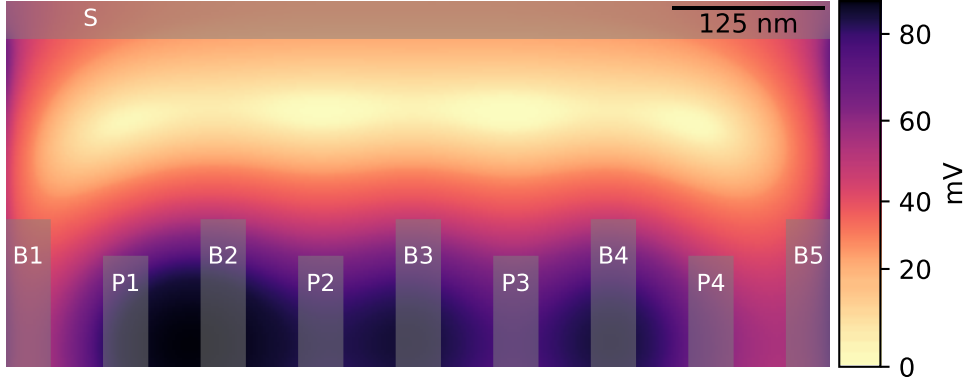


Figure 3.1: Confinement potential of four quantum dots in the plane of 2DEG. Plunger gates (P1, P2, P3, and P4) are used to tune the chemical potential of each dot, and barrier gates (B2, B3, and B4) are used to tune the interdot tunnel couplings. The screening gate (S) forms a tunnel barrier between the qubit dots and sensor dots (not shown in the image). Gates B1 and B5 control the electron tunneling rate between a corner dot and a neighboring electron reservoir.

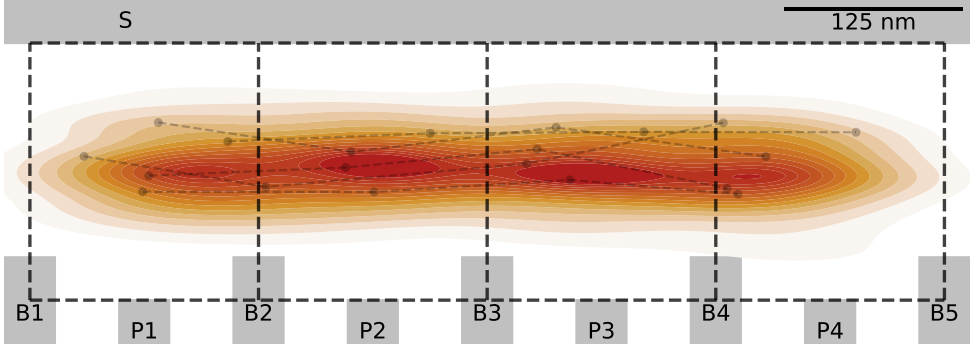


Figure 3.2: The distribution of dot centers in the samples converged after numerical optimization. Dots connected by dashed lines are the representatives of converged realizations. Each dot is localized to its expected region which is shown by dashed rectangular boxes. Gate profiles are shown similar to Fig. 3.1.

realizations, we find that most measured gate coupling strengths and gate voltages lie within the standard deviation of the computed ones.

3.3.2. NON-PLANAR GEOMETRY

To demonstrate the universality of our approach, we calculate the gate coupling strengths in a non-planar geometry. We consider the Si-heterostructure from Ref. [17, 30]. This device consists of a slab of Si grown on an insulator as shown in Fig. 3.5. The Si is surrounded by SiO₂ on the four faces with plunger and barrier gates deposited on the top, right, and left faces. We tune the gates on one side of the device to form quantum dots underneath. The other side is used for sensing and plays no role in our simulations. Similar to the planar geometry, the plunger gates P1, P2, and P3 control the dot occupation, while the barrier gates B2 and B3 tune the tunnel barrier strengths. We apply the optimization

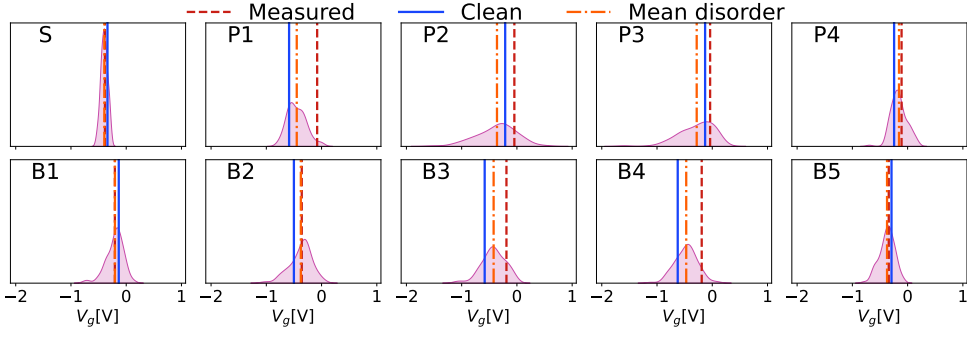


Figure 3.3: Comparison of gate voltages between the experiment (dashed line) from Ref. [28] and simulation. The distribution of gate voltages for the converged disordered samples is shown. Voltages of the clean system and the mean of the distribution in the disordered case are also shown by solid and dash-dotted lines respectively.

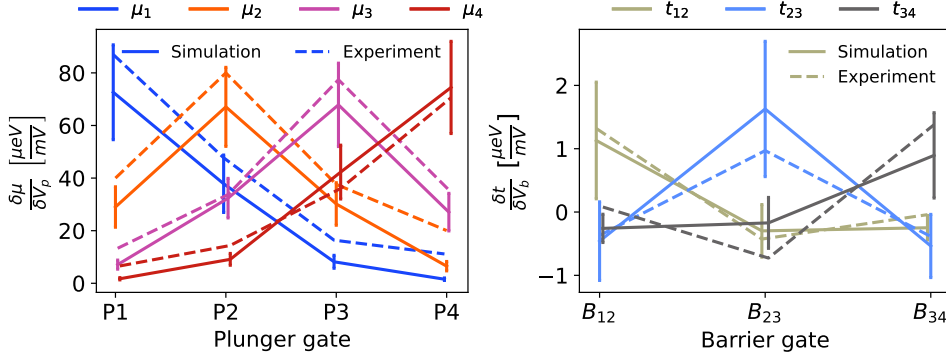


Figure 3.4: Numerically calculated gate coupling strengths in GaAs heterostructure compared against the measurements from [28]. Solid lines represent the numerical results whereas dashed lines represent the measured data. The mean of the distribution of gate coupling strengths corresponding to the samples converged after numerical optimization is plotted and the error bars indicate the standard deviation. Coupling strengths from plunger gates to the chemical potential of four dots and barrier gates to the interdot tunnel couplings are shown in the left and right panels respectively.

procedure of Sec. 3.2 to tune the device to its operating point. Due to the device geometry, electron wave functions localize near the sample edge under the plunger gates as shown in Fig. 3.5.

We simulate disorder in the Si potential landscape by randomly distributing positive charges in SiO₂ with a surface charge density of $7.5 \times 10^{10} \text{ cm}^{-2}$ which is close to the experimentally observed value in the SiO₂ [33] and we perform numerical optimization in two stages. Due to the larger effective mass in Si, the tuning of the non-planar device is less stable. We resolve this by excluding the contribution of interdot coupling to $f'(V)$ in the first optimization step. In the second step, we optimize $f(V)$ with $t_0 = 5 \mu\text{eV}$. We repeat this process for 200 realizations of surface charge disorder. After the two-stage optimization, we compute the gate coupling strengths using Eq. (3.8) only for those

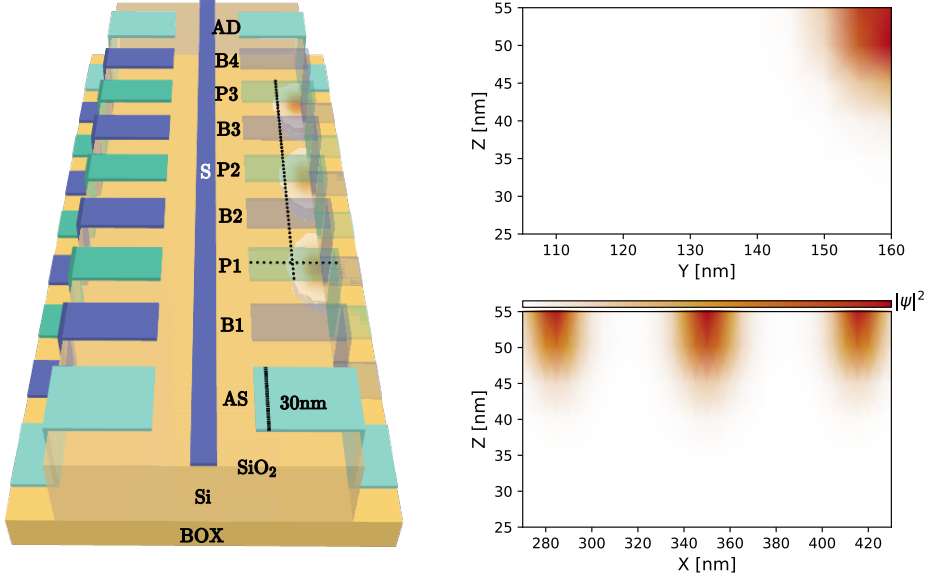


Figure 3.5: Silicon spin-qubit device with non-planar gate geometry. Si is surrounded on four faces by SiO₂ which electrically isolates Si from the gate electrodes. Plungers (P1, P2, and P3) and accumulation (AS and AD) gates are mainly used to accumulate electrons underneath them in Si whereas barrier gates (B1 to B4) are mainly used to form a tunnel barrier between the dots. A similar set of gates shown on the left side of the device is used to form sensor dots. Gate S is used to control the electrostatic coupling between qubits and sensor dots for charge sensing. The probability density of the bound state in three dots on the right channel is shown. Longitudinal cross-section across gates P1 to P3 and lateral cross-section beneath the gate P1 is shown on the right.

samples for which the optimization converges with precision $|\alpha - 1| < 0.01$, $|\mu_i| < 50 \mu\text{eV}$ and $|t_{ij} - t_0| < 0.5 \mu\text{eV}$. Finally, we filter out several outlier disorder realizations with $\delta|t_{ij}|/\delta V > 10 \mu\text{eV}/\text{mV}$. After performing the two filtering steps, just over 50 % of realizations remain. In Fig. 3.6, we show the plunger and barrier gate coupling strengths to the dot chemical potential and interdot tunnel couplings for the filtered realizations. We find that due to the stronger localization of the wave functions and the smaller distance between the gates and the bound states, the non-local gate couplings are strongly suppressed in the non-planar geometry, compared to the planar one.

3.4. SUMMARY

We developed a software tool to predict the disorder-induced variation in spin qubit devices. Our approach relies on an automated tuning procedure able to tune devices with realistic disorder in the majority of disorder realizations to their operating point. To benchmark our result, we compared the predicted gate voltage and gate coupling strengths distributions to those measured in a GaAs device and found an agreement within a standard deviation of the predicted parameters. We demonstrated that our tool also functions with a comparable efficiency when applied to a non-planar Si device.

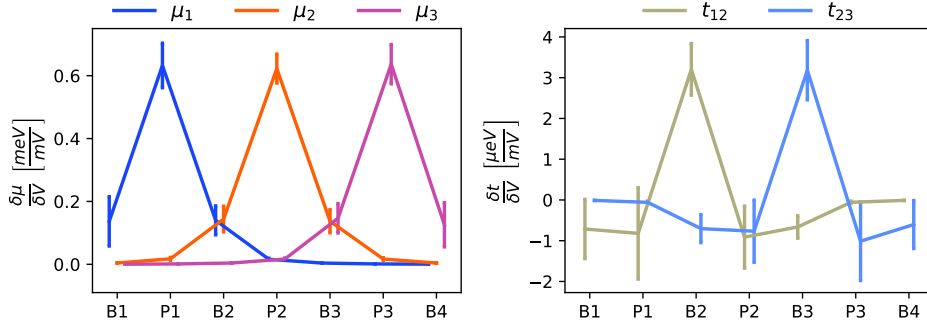


Figure 3.6: Numerically calculated gate coupling strengths of non-planar geometry. Gate coupling strengths to the chemical potential of three dots and the interdot tunnel couplings are shown in the top and bottom panels respectively. The asymmetric uncertainty in the gate coupling strengths to μ_1 and μ_3 is because the barrier and accumulation gates at the edges of the device are not constrained in the numerical optimization.

Currently, our package disregards interdot Coulomb repulsion as well as lattice strain. We expect that after extending the simulation to include these phenomena in the simulation, our approach will become sufficiently general to optimize device geometry and guide the tuning of experimentally realized devices.

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Data Availability All code and data used in the manuscript are available at Zenodo [29].

Author contributions S.R.K. and A.A. formulated the project goal with input from L.W.; A.A. and S.R.K. designed the project approach; S.R.K. and H.K. established electrostatic simulations with input from C.X.L.; under the supervision of A.A., S.R.K. and H.K. carried out numerical simulations of the planar and the non-planar geometry respectively; S.R.K., C.X.L., and A.A. interpreted the results; S.R.K., H.K., and A.A. wrote the manuscript with input from C.X.L. and L.W.

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4

DESIGN OF A MAJORANA TRIJUNCTION

This chapter has been previously published as Juan Daniel Torres Luna, Sathish R. Kuppuswamy, and Anton Akhmerov, *Design of a Majorana trijunction*. Together with Juan Daniel Torres Luna, I set up the simulations and explored gate voltage space with numerical optimization. I calculated the Majorana trijunction performance in presence of disorder. I added corresponding plots to the manuscript and supported Juan Daniel Torres Luna in writing manuscript.

4.1. INTRODUCTION

A pair of well-separated Majorana states encode the occupation of a single fermionic state non-locally as two zero-energy states [1]. Under the exchange of two Majorana states, the protected ground state evolves via unitary operations. The discrete nature of braiding allows the implementation of all Clifford operations with very low error rates—a requirement for universal fault-tolerant quantum computation [2]. This has brought a lot of attention to the field in the past two decades with several proposals for experimental realization [3, 4] and detection [5–7] of Majorana bound states. Therefore, several proposals for braiding include moving Majoranas around each other in semiconductor nanowire networks [8, 9], long-range coupling of Majorana islands connected by quantum dots [10–13], and networks of Josephson junctions connected by trijunctions [14, 15].

Braiding in hybrid semiconductor-superconductor devices requires coupling all Majorana states via control of the electrostatic potential. Two-dimensional electron gases (2DEGs) are suitable for realizing trijunction devices because they combine different ingredients such as electrostatic control and superconductivity [4] in a non-linear layout. 2DEGs are an active field of research for topological physics with experiments focused on detecting signatures of Majorana states in single nanowires [16–18], planar Josephson junctions [19, 20], or in minimal realizations of the Kitaev chain [21, 22]. Unambiguous detection of Majoranas requires distinguishing them from non-Majorana physics producing similar results [23, 24]. The recently proposed topological gap protocol [7] establishes a first step toward fully automated detection of Majorana states.

A braiding experiment poses additional requirements to the creation of spatially isolated Majoranas. It requires measurement of the fermion parity of Majoranas belonging to the same nanowire [25, 26]. Furthermore, it also requires a trijunction—a switch that selectively couples Majoranas from three different nanowires—which is the focus of our work. The requirements for a braiding experiment are such that (i) the energy of the coupled pairs needs to be larger than the thermal broadening, (ii) the ratio of the energies of coupled pairs with the remaining Majoranas should be as large as possible to ensure adiabaticity, and (iii) the gap between the zero-energy ground state and the coupled Majoranas does not close while coupling different pairs. A trijunction device that satisfies these requirements is suitable to perform braiding.

To evaluate the feasibility of a braiding experiment, we design and simulate a trijunction device as shown in Fig. 4.1. To find the operational regime of the device, we use an optimization approach using an effective Hamiltonian in the basis of decoupled Majorana states. Then, we illustrate the device operation by simulating the braiding protocol from Ref. [15] where we switch the coupling between different pairs of Majorana states while preserving the energy gap. We define quality metrics relevant for braiding and systematically compare the performance of different trijunction device geometries. We highlight the geometries that are suitable for braiding and investigate their resilience to increasing concentration of electrostatic disorder that is unavoidable in this system [7].

4.2. DEVICE LAYOUT AND BRAIDING PROTOCOL

A braiding protocol [15, 27] requires time-dependent manipulation of the pair couplings between three Majorana states shown in Fig. 4.1 (a). The computational subspace—one

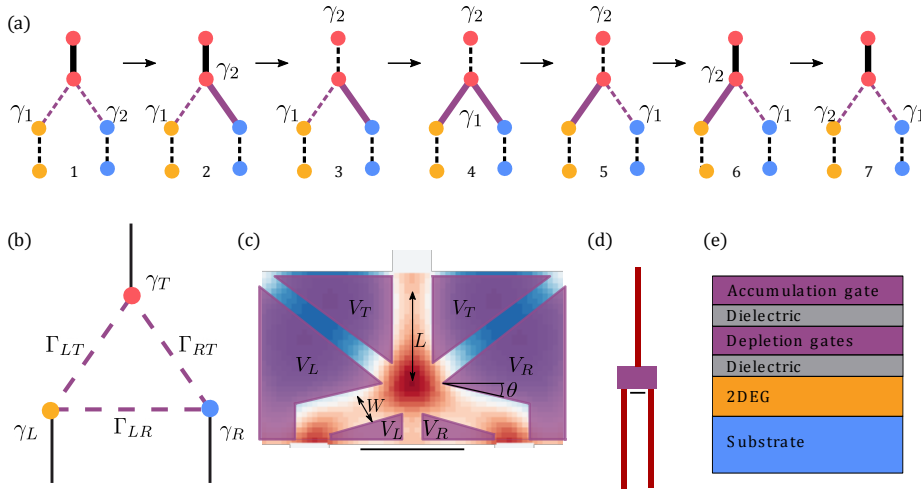


Figure 4.1: (a) The braiding protocol that we consider [15]. The lines indicate Majorana couplings that are either on (thick lines) or off (dashed lines). (b) A schematic of a trijunction device showing three Majorana states closest to the trijunction region (red, blue, and yellow) and their pairwise couplings. (c) Real space trijunction layout. The shape of the depletion gates (purple) is parametrized by L , W , and θ . The background color shows the chemical potential. Blue regions are depleted and red regions are not. The scale bar is 200 nm. (d) The complete simulated device. The trijunction is in the middle (purple rectangle), with the nanowires (red lines) attached to it. (e) Heterostructure configuration.

Majorana in the trijunction and three Majoranas in the far nanowires' ends—is protected as long as the number of zero-energy modes remains constant. In other words, the computation is protected as long as two out of six Majorana states are always coupled. The full braiding protocol requires coupling Majoranas from the same wire via a transmon [26] or flux qubit [25], which is outside the scope of this work. It also requires moving one Majorana state between three different wires by coupling different pairs of Majoranas via a trijunction. By combining these two procedures, it is possible to perform a braiding experiment where two Majorana states exchange positions.

We adapt the braiding protocol from Ref. [15] that exchanges Majoranas γ_1 and γ_2 as shown in Fig. 4.1 (a). The ingredients that we require for the braiding protocol are

- coupling Majoranas within the same nanowire via charging energy [25, 26],
- coupling pairs of Majoranas via the trijunction,
- coupling all three Majoranas in the trijunction as in step 5 of Fig. 4.1 (a),
- a path in parameter space that interpolates between a regime with two Majoranas coupled to the regime with three Majoranas coupled without closing the topological gap, that is, a path with a finite gap during steps 3, 4, and 5 of Fig. 4.1 (a).

Our goal is to compute the coupling of different Majoranas required to implement the braiding protocol of Fig. 4.1 (a). Because the purpose of our study is the design of the trijunction, we exclusively consider the three Majoranas closest to the trijunction which

interact via the potential in the middle region shown in Fig. 4.1 (c). Therefore, we do not consider the Coulomb couplings between the Majoranas in the nanowires shown in steps 1 and 7 in Fig. 4.1 (a). For the same reason, we leave to future work the competition between Coulomb-mediated Majorana coupling and the direct coupling at the trijunction [28]. Furthermore, because the on/off ratios of the couplings are sufficient to determine the adiabaticity of the braiding protocol, we do not simulate the explicit time dependence of gate voltages. Finally, detailed modeling of Majorana nanowires is outside the scope of our study. Therefore, we consider an idealized model of topological nanowires.

We simulate clean nanowires of size $W_{NW} = 70 \text{ nm}$ and $L_{NW} = 1.5 \mu\text{m}$ such that the Majoranas are well-separated. An external magnetic field is parallel to the nanowires and drives them into the topological phase. We connect the nanowires to the trijunction formed in the central normal region as shown in Fig. 4.1 (c). We use one layer of depletion gates shown in Fig. 4.1 (c) to form the trijunction and a second layer for a global accumulation gate to control the electron density. We parameterize the shape of the device using channel length L , channel width W , and the angle θ between the x -axis and the arms. We use the materials from Ref. [29] for the substrate, dielectric, and gate electrodes.

We simulate the three-dimensional device configuration shown in Fig. 4.1 (c-e). We use the electrostatic solver of Ref. [30] to numerically solve the Poisson's equation

$$\nabla \cdot [\epsilon_r(\mathbf{r}) \nabla U(\mathbf{r})] = -\frac{\rho(\mathbf{r})}{\epsilon_0}, \quad (4.1)$$

where ρ_r is the charge density, ϵ_0 is the vacuum permittivity and ϵ_r is the relative permittivity. Because the 2DEG has a low electron density, we neglect the potential induced by charges in the 2DEG. We express U as a linear combination of the potential induced by each gate electrode

$$U(\mathbf{r}) = \sum_i V_i U_i(\mathbf{r}) + U_0(\mathbf{r}), \quad (4.2)$$

where $U_0(\mathbf{r})$ is the potential induced by dielectric impurities when $\mathbf{V} = 0$, and V_i are the elements of $\mathbf{V} = (V_L, V_R, V_T, V_{\text{global}})$. To reduce the number of control parameters, we apply the same voltages to the depletion gates closest to a channel shown in Fig. 4.1 (c).

We use the 2D Hamiltonian

$$H = \left(\frac{1}{2m^*} (\partial_x^2 + \partial_y^2) - U(x, y) \right) \sigma_0 \tau_z + \alpha (\partial_x \sigma_y - \partial_y \sigma_x) \tau_z + E_z \sigma_y \tau_0 + \Delta(x, y) \sigma_0 \tau_x, \quad (4.3)$$

where σ_i and τ_i are the Pauli matrices in the spin and particle-hole space, α is the spin-orbit coupling strength, E_z is the Zeeman field induced by the homogeneous magnetic field, and m^* is the effective mass in the semiconductor. Using the Kwant software package [31], we discretize Eq. (4.3) over a 2D tight-binding square lattice with lattice constant $a = 10 \text{ nm}$ as for typical devices [32]. The electrostatic potential in the 2DEG, $U(x, y, z = 0) = U(x, y)$, is defined relative to the Fermi level in the nanowires which is set to the bottom of the lowest transverse band μ . The superconducting pairing is absent in the normal region, and in the nanowires, it is $\Delta(x, y) = \Delta_0 e^{i\phi_j}$ where Δ_0 is the induced gap and ϕ_j is the phase in the j -th nanowire. We tune the Hamiltonian to be in the topological phase for the lowest subband, $E_z > \sqrt{\mu^2 + \Delta_0^2}$. The topological gap in the nanowires is Δ_t . The parameters used in the Hamiltonian and the electrostatic simulation are listed in Appendix .1.

4.3. DEVICE TUNING

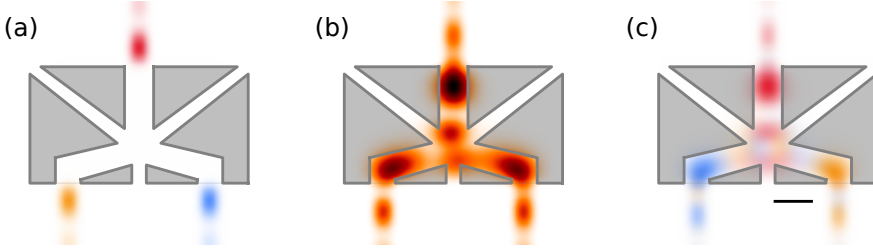


Figure 4.2: Representation of coupled Majoranas in the basis of localized states. (a) Densities of 3 decoupled Majorana states $|\gamma_i\rangle$. (b) wave function of coupled Majoranas $|\psi_j\rangle$. (c) Decomposition of the coupled wave function into decoupled states using the SVD.

4

To determine couplings of individual Majoranas from the low-energy eigenvalue decomposition of the Hamiltonian, we need to interpret the wave functions in terms of Majoranas belonging to different wires. We do this by first considering a point in the parameter space where the trijunction is disconnected and use it to define the reference Majorana wave functions. We numerically compute the six lowest energy modes $|\phi_i\rangle$ of the full device shown in Fig. 4.1 (d) when the normal region is depleted. The eigenstates $|\phi_i\rangle$ are linear combinations of decoupled Majorana states $|\gamma_i\rangle$. We obtain a basis of individual Majorana states $|\gamma_i\rangle = \hat{W}|\phi_i\rangle$, where $\hat{W}$ is the matrix that simultaneously approximately diagonalizes the projected position operators $\hat{\mathbf{P}}_x = \langle\phi_i|\hat{\mathbf{X}}|\phi_j\rangle$ and $\hat{\mathbf{P}}_y = \langle\phi_i|\hat{\mathbf{Y}}|\phi_j\rangle$. After Wannierization, we fix the phase of $|\gamma_i\rangle$ so that $\mathcal{P}|\gamma_i\rangle = |\gamma_i\rangle$ so they are particle-hole symmetric. To determine the effective trijunction Hamiltonian, we project out the decoupled Majorana states at the far ends of the wires and keep only the Majorana states that are closest to the middle region, as shown in Fig. 4.2 (a). When the three Majoranas are strongly coupled as in Fig. 4.2 (b), the eigenstates $|\psi_j\rangle$ are not linear combinations of decoupled Majorana states. However, the three eigenstates closest to the trijunction form a particle-hole symmetric subspace where any fermionic state can be expressed as a linear combination of the individual Majorana states $|\gamma_i\rangle$ as in Fig. 4.2 (c).

We interpret the coupled eigenstates as linear combinations of Majoranas originating from different arms by using the overlap between the i -th decoupled and j -th coupled Majoranas, $S_{ij} = \langle\gamma_i|\psi_j\rangle$. We then apply a singular value decomposition (SVD), $S = UDV^\dagger$, where U and V are unitary and D is a positive diagonal. The approximate transformation is the unitary part of the SVD, $S' = UV^\dagger$. This transformation corresponds to choosing the coupled Majorana wave functions as $|\gamma'_j\rangle = \sum_k S'_{jk}|\psi_k\rangle$ as shown in Fig. 4.2 (b-c). The low-energy effective Hamiltonian is

$$H_{\text{eff}} = S' \text{diag}(-E_1, 0, E_1) S'^\dagger = i \sum_{i \neq j} \Gamma_{ij} |i\rangle \langle j|, \quad (4.4)$$

where $\Gamma_{ij} = -\Gamma_{ji}$ is the coupling between Majoranas γ'_i and γ'_j , and E_1 is the energy of the first excited state of the system. When only two Majoranas are coupled, their effective coupling $|\Gamma_{ij}| = E_1$, however, when there are multiple pairs of coupled Majoranas, the interpretation of the effective couplings Γ_{ij} is ambiguous.

4.4. OPTIMIZING PAIRWISE COUPLINGS

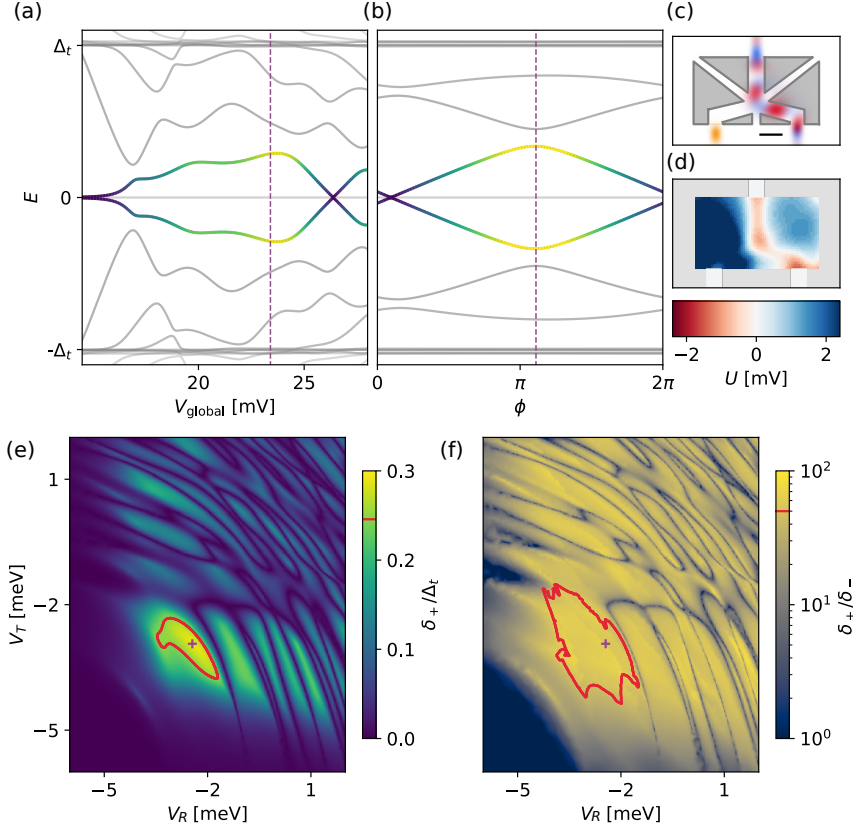


Figure 4.3: Spectra of a trijunction with optimally coupled $R - T$ pair of Majoranas (colored lines) with respect to (a) global accumulation gate and (b) superconducting phase difference. The optimal point is indicated by the purple dashed lines. The wave functions (c) and the potential (d) at the optimal point. Two-dimensional scans as a function of the voltages for the T and R depletion gates of the desired coupling (e) and the ratio of desired over undesired coupling (f). The optimal point is shown as a purple cross inside of the scan. The operation range is shown as a red line that corresponds to the area with $\delta_+ \leq 0.85 \times \delta_+^{\max}$ and $\delta_+ / \delta_- > 50$.

Initially, we consider steps 2, 3, 5, and 6 of Fig. 4.1 (a) where a single pair of Majoranas is connected via the trijunction. We use an optimisation approach to find the optimal couplings as a function of gate voltages and phase differences. For the coupling of the i -th and j -th Majorana states, we define the desired and undesired couplings as

$$\delta_+ = |\Gamma_{ij}|, \quad \delta_- = |\Gamma_{ik}| + |\Gamma_{jk}|, \quad (4.5)$$

where k is the remaining Majorana state. The goal of our device is to maximize the energy of the coupled Majorana pair while keeping the couplings to the remaining Majorana state exponentially small. Therefore, we define a loss function that maximizes the desired

coupling and minimizes the undesired coupling:

$$C_{\text{pair}} = -\delta_+ + \log(\delta_-^2 + \epsilon). \quad (4.6)$$

Here, $\delta_{\pm}$ is in units of Δ_t . We use $\epsilon = 10^{-3}$ to regularize the divergence of the logarithm.

To remove the local minima of the loss function and improve the convergence, we penalize the regions in the gate voltage space where either the regions under the gate are not depleted or the channels are fully depleted. We achieve this by adding the following soft-threshold terms to the loss function:

$$S(U(\mathbf{r})) = A \left(\sum_{\{\mathbf{r}_{\text{acc}}\}} U(\mathbf{r}_{\text{acc}}) \Theta[U(\mathbf{r}_{\text{acc}})] + \sum_{\{\mathbf{r}_{\text{dep}}\}} (U(\mathbf{r}_{\text{dep}}) - u_0) \Theta[-U(\mathbf{r}_{\text{dep}})] \right). \quad (4.7)$$

Here $\Theta(x)$ is the Heaviside function. We choose $\{\mathbf{r}_{\text{acc}}\}$ and $\{\mathbf{r}_{\text{dep}}\}$ to be in the accumulated channel and in the depleted regions, respectively. We choose the scale factor $A = 10^2$, and use a threshold $u_0 \sim 1 - 2$ meV. The total loss function is

$$L = C_{\text{pair}} + S. \quad (4.8)$$

Minimizing this loss function for all Majorana pairs yields the voltage configurations where two Majorana states are optimally coupled. The results for the R - T pair are shown in Fig 4.3. At the optimal point, the depletion gates form a channel between the R and T Majorana states while disconnecting the L Majorana as shown in Fig. 4.3 (c-d). Once the channel is formed by the depletion gates, the coupling is controlled by tuning the accumulation gate voltage V_{global} as shown in Fig. 4.3 (a). The phase difference between the top and right superconducting arms modulates the coupling Γ_{LR} as shown in Fig. 4.3 (d).

4.5. OPTIMIZING TRIPLE COUPLING

To couple all three Majorana states, at least two pairs of Majoranas must be coupled. Because the device without disorder is symmetric around the x axis, we choose to couple the L - T and R - T pairs of Majoranas simultaneously, and constrain the voltages to be symmetric, i.e. $V_L = V_R$. Furthermore, since finding the optimal path in voltage space is hard, we choose the path that linearly interpolates between the point where two Majorana states are coupled and the point where all Majorana states are coupled, corresponding to steps 3, 4, and 5 of Fig. 4.1 (a). To find a triple-coupled point, the loss function must maximize at least two couplings simultaneously. Furthermore, depending on the choice of the triple coupled point, the gap along the path interpolating between the pairwise coupling and the triple point may close. In the trijunction that we have studied, we find that the following loss function finds a triple coupled point connected by a gapped path to the pair of coupled points:

$$C_{\text{triple}} = -(|\Gamma_{LT}| + |\Gamma_{RT}|) + |\Gamma_{LR}|. \quad (4.9)$$

The gap reaches a minimum $\approx 0.1 \times \Delta_t$ along the braiding path. We obtain the optimal coupling by minimizing the loss function as in Eq. (4.9) plus the corresponding soft-threshold to accelerate convergence. The resulting spectrum of the trijunction has a finite gap during the entire voltage path as shown in Fig. 4.4. The wave functions at the optimal points are shown in the upper row of Fig. 4.4.

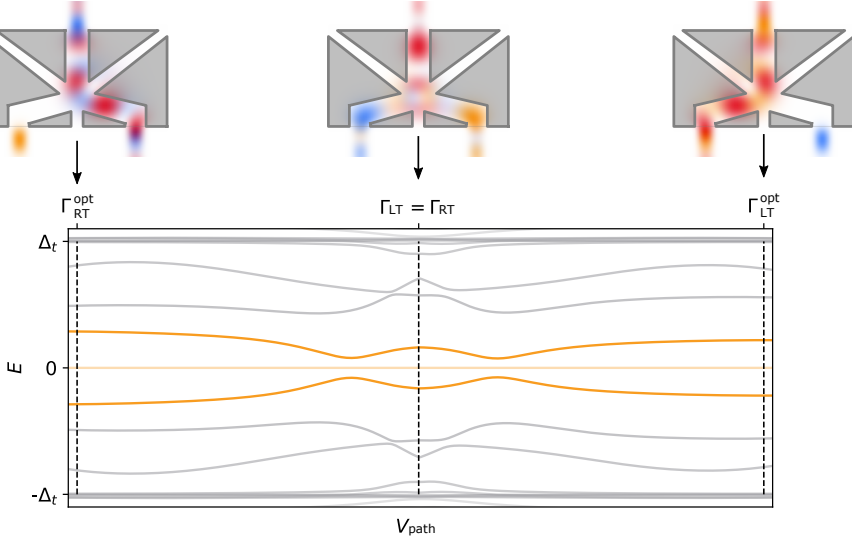


Figure 4.4: Exchange of two Majoranas by adiabatically coupling different pairs of Majoranas. (Top) Majorana wave functions at the optimal points where one or two pairs of Majoranas are coupled. (Bottom) The spectrum of the trijunction along the voltage path that interpolates between the optimal points.

4.6. GEOMETRY DEPENDENCE

To evaluate the adiabaticity of the braiding protocol, we compute the desired coupling, δ_+ , and the ratio between desired and undesired couplings, δ_+/δ_- , at the optimal point. Because the topological gap is small, we require the Majorana couplings to be comparable to it:

$$\delta_+ \gtrsim 0.3 \times \Delta_t. \quad (4.10)$$

As a minimum requirement for adiabaticity, the desired coupling should be larger than the undesired coupling:

$$\delta_+ \gtrsim 50 \times \delta_-. \quad (4.11)$$

The large ratio between desired and undesired couplings ensures that there exists a time scale τ where the device operates such that $\delta_- < \hbar/\tau < \delta_+$. Furthermore, the coupling δ_+ must be larger than the thermal broadening. While at the optimal point, δ_+ and δ_+/δ_- are optimal, device operation depends on the stability of these values with respect to variations in the gate voltages. Therefore, we define the operational range $\mathcal{A}$ of the device as the area in the voltage space that satisfies both Eqs. (4.10) and (4.11). In Fig. 4.3 (e-f) we show the operational regime of the device around the optimal point for the desired coupling and the ratio between the desired and undesired couplings, respectively. While the numerical values of the thresholds are somewhat arbitrary, they leave sufficient room for adiabatic braiding while not introducing additional limitations to the device's performance.

To determine which geometries are suitable for braiding, we compute the quality metrics δ_+/Δ_t , δ_+/δ_- , and $\mathcal{A}$ for different L , W , and θ . We evaluate the quality metrics for the worst-performing pair. We summarize the results in Fig. 4.5 and indicate the

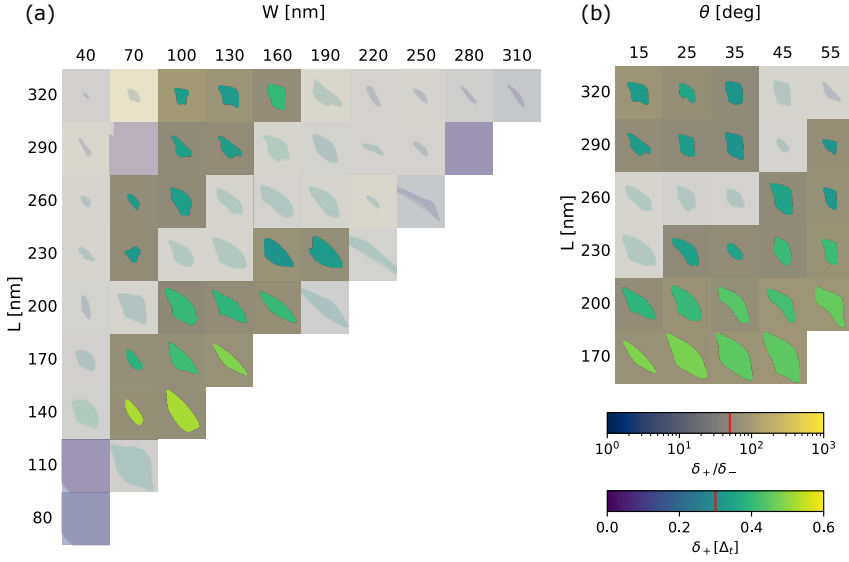


Figure 4.5: Analysis of quality metrics for the worst performing pair for different trijunction geometries with $\theta = 15^\circ$ (left) and $W = 130$ nm (right). The operation range for each geometry is shown inside each square and colored with δ_+ at the optimal point. The background is colored with δ_+ / δ_- at the optimal point. The optimality criteria from Eqs. (4.10) and (4.11) is indicated by a red line in the respective color bar. The geometries that do not satisfy these criteria have increasing transparency. The squares fully covered in purple are the cases when the optimization algorithm did not find a solution.

geometries that meet the thresholds in Eqs. (4.10) and (4.11). We find that the quality of a trijunction depends on the length scales of the normal region. Because Majorana couplings decay with distance, small trijunctions have a systematically larger operational voltage range. In very small trijunctions, however, it becomes impossible to suppress unwanted couplings. Furthermore, there is an optimal aspect ratio between length L and width W that guarantees control over the individual channels formed in the trijunction arms. The angle θ does not affect the qualitative behavior of the trijunction.

4.7. ELECTROSTATIC DISORDER

We compare the susceptibility to electrostatic disorder of larger and smaller geometries. For that, we select two geometries and analyze their performance in the presence of disorder. We simulate disorder in the dielectric between the depletion gate layer and 2DEG by randomly positioned positive charges. Figure 4.6 shows that devices with an impurity concentration of $\sim 10^{10} \text{ cm}^{-2}$ are not degraded by disorder. On the other hand, a small concentration of electrostatic disorder $\sim 10^{11} \text{ cm}^{-2}$, which is reported to be achieved in Ref. [7], significantly reduces the performance of a trijunction. While smaller geometries perform better, we expect that they are more susceptible to fabrication imperfections, therefore posing a tradeoff between two challenges.

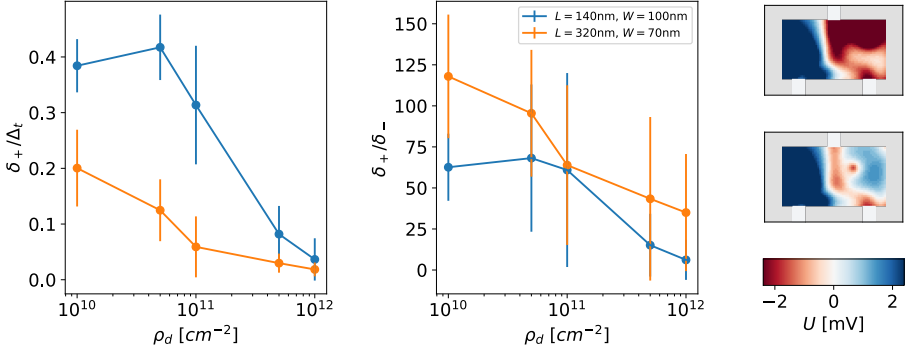


Figure 4.6: Impact of disorder on δ_+ (a) and δ_+/δ_- (b). We show two example disordered realizations (c) for $\rho = 10^{10} \text{ cm}^{-2}$. We considered 10 disorder realizations for each impurity density. The error bars correspond to the standard deviation.

4

4.8. SUMMARY

In this work, we developed a numerical procedure to design a braiding protocol using a trijunction device—one of the ingredients for a topologically protected quantum computer—by using three-dimensional electrostatic and quantum simulations. We used an optimization approach to find the voltage configurations where all different pairs of Majorana states are strongly coupled. Consequently, we discovered that a range of trijunction device geometries can be used as switches that selectively couple and decouple different Majorana states. We confirmed that trijunctions are suitable for braiding by simulating the braiding protocol from Ref. [15] without closing the gap between the ground state and the coupled Majorana states. The operation of the device is limited by the gap size, which decreases to $\lesssim 0.1 \times \Delta_t$ along the braiding protocol. We observe that state-of-the-art levels of disorder render this trijunction design inoperable because the narrow channels cannot be formed. Therefore, we expect that cleaner materials [33] or a different design would be required to resolve this problem.

The methods developed in our study apply to other realizations of Majorana states such as the minimal Kitaev chain [21, 34]. Similarly, the optimization method that we developed is transferable to other semiconducting devices such as spin qubits [35], or hybrid devices such as planar Josephson junctions [32]. The operational regime of these devices usually lies in a region of a multidimensional space that maximizes certain quantities such as the wave function overlap [35] or the energy gap [32]. Our work demonstrates that combining electrostatic simulations, effective Hamiltonians, and optimization routines is a powerful tool for designing and operating semiconductor devices.

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Author contributions A.R.A. defined the project goal and supervised the project. J.D.T.L. designed the trijunction device. J.D.T.L. and S.R.K. set up the simulations and obtained the results. J.D.T.L. wrote the manuscript with input from S.R.K. and A.R.A.

Data availability All code and data used in this work are available at Ref. [36].

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.1. SIMULATION DETAILS

The values used in Eq.(4.3) are $t = \hbar^2/2m^*$ where $m^* = 0.023 \times m_e$ and m_e is the electron mass, the bare superconducting gap is $\Delta_0 = 0.5 \text{ meV}$, the spin-orbit interaction $\alpha = 3 \times 10^{-11} \text{ eVm}$, the Zeeman field that drives the nanowires in the topological phase is $E_Z = 1.0 \text{ meV}$, and the nanowire chemical potential at the bottom of the lowest band is $\mu = 2.396 \text{ meV}$. The topological gap is $\Delta_t = 0.325 \text{ meV}$. The coherence length in the nanowires is $\xi_{sc} \approx 80.2 \text{ nm}$ and the localization length of the Majoranas is $\xi_{\text{MZM}} \approx 487.474 \text{ nm}$. Similarly, in Table 1 we detail the parameters used to set up the three-dimensional electrostatic simulation and solve Eq.(4.1).

Layer	Thickness [nm]	Relative permittivity
Substrate	50	16
2DEG	20	15
Dielectric	30	9.1

Table 1: Parameters used in the electrostatic simulations. The heterostructure layers are shown in Fig.4.1(c) and their corresponding thicknesses and relative dielectric permittivities with respect to the vacuum permittivity ϵ_0 are detailed here. The metallic gates have infinite permittivity and a thickness of 30 nm.

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LIST OF PUBLICATIONS

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2. **Sathish R. Kuppuswamy**, Hugo Kerstens, Chun-Xiao Liu, Lin Wang, Anton Akhmerov, *Impact of disorder on the distribution of gate coupling strengths in a spin qubit device*, arXiv:2208.02190 (2022).
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